

Table 1

**NMR Chemical
Shift Assignment
of the P/CAF
Bromodomain**

RES_ID 715
RES_TYPE GLY
SPIN_SYSTEM_ID 1
HETEROGENEITY 100
END_RES_DEF

RES_ID 716
RES_TYPE SER
SPIN_SYSTEM_ID 2
HETEROGENEITY 100
END_RES_DEF

RES_ID 717
RES_TYPE HIS
SPIN_SYSTEM_ID 3
HETEROGENEITY 100
END_RES_DEF

RES_ID 718
RES_TYPE MET
SPIN_SYSTEM_ID 4
HETEROGENEITY 100
END_RES_DEF

RES_ID 719
RES_TYPE SER
SPIN_SYSTEM_ID 5
HETEROGENEITY 100
END_RES_DEF

RES_ID 720
RES_TYPE LYS
SPIN_SYSTEM_ID 6
HETEROGENEITY 100
CA 56.296000
HA 4.361000
CB 33.140000
HB1 1.882000
HB2 1.684000
CG 25.430000
HG1 1.585000
HG2 1.433000
CD 29.834000
HD1 1.703000
CE 41.960000
HE1 3.003000
END_RES_DEF

RES_ID 721
RES_TYPE GLU
SPIN_SYSTEM_ID 7
HETEROGENEITY 100
N 122.990000
HN 8.317000
CA 54.620000
HA 4.540000
CB 29.830000
HB1 2.024000
HB2 1.893000
CG 35.893000
HG1 2.271000
END_RES_DEF

RES_ID 722
RES_TYPE PRO
SPIN_SYSTEM_ID 8
HETEROGENEITY 100
CA 63.430000
HA 4.393000
CB 32.030000
HB1 2.224000
HB2 1.880000
CG 27.630000
HG1 2.028000
CD 50.760000
HD2 3.656000
HD1 3.800000
END_RES_DEF

RES_ID 723
RES_TYPE ARG
SPIN_SYSTEM_ID 9

HETEROGENEITY 100
N 121.192000
HN 8.416000
CA 63.430000
HA 4.331000
CB 30.930000
HB1 1.815000
HB2 1.762000
CG 27.630000
HG1 1.681000
CD 43.603000
HD1 3.161000
END_RES_DEF

RES_ID 724
RES_TYPE ASP
SPIN_SYSTEM_ID 10
HETEROGENEITY 100
N 122.012000
HN 8.273000
CA 52.415000
HA 4.874000
CB 41.400000
HB1 2.754000
HB2 2.692000
END_RES_DEF

RES_ID 725
RES_TYPE PRO
SPIN_SYSTEM_ID 11
HETEROGENEITY 100

CA 65.080000
HA 4.329000
CB 32.590000
HB1 2.326000
HB2 1.973000
CG 27.632000
HG1 2.028000
CD 51.310000
HD1 3.866000
END_RES_DEF

RES_ID 726
RES_TYPE ASP
SPIN_SYSTEM_ID 12
HETEROGENEITY 100
N 119.716000
HN 8.397000
CA 55.720000
HA 4.692000
CB 40.550000
HB1 2.792000
HB2 2.730000
END_RES_DEF

RES_ID 727
RES_TYPE GLN
SPIN_SYSTEM_ID 13
HETEROGENEITY 100
N 121.356000
HN 8.196000
CA 55.920000
HA 4.163000
CB 28.730000
HB1 2.148000
CG 34.240000
HG1 2.524000
HG2 2.371000
END_RES_DEF

RES_ID 728
RES_TYPE LEU
SPIN_SYSTEM_ID 14
HETEROGENEITY 100
N 121.356000
HN 8.210000
CA 58.473000
HA 4.045000
CB 41.400000
HB1 1.847000
HB2 1.555000
CG 27.080000
HG 1.480000
CD1 25.970000
HD1# 0.794000
CD2 23.226000
HD2# 0.786000
END_RES_DEF

RES_ID 729
RES_TYPE TYR
SPIN_SYSTEM_ID 15
HETEROGENEITY 100
N 119.060000
HN 8.021000

CA 62.320000
HA 4.038000
CB 38.640000
HB1 3.211000
HB2 3.024000
CD1 134.350000
HD1 7.053000
CE1 119.481000
HE1 6.882000
END_RES_DEF

RES_ID 730
RES_TYPE SER
SPIN_SYSTEM_ID 16
HETEROGENEITY 100
N 112.173000
HN 8.167000
HA 3.920000
HB1 3.995000
END_RES_DEF

RES_ID 731
RES_TYPE THR
SPIN_SYSTEM_ID 17
HETEROGENEITY 100
N 120.372000
HN 8.059000
CA 66.730000
HA 3.924000
CB 68.930000
HB 4.247000
CG2 21.570000
HG2# 1.142000
END_RES_DEF

RES_ID 732
RES_TYPE LEU
SPIN_SYSTEM_ID 18
HETEROGENEITY 100
N 120.536000
HN 8.460000
CA 57.920000
HA 3.289000
CB 39.750000
HB1 1.532000
HB2 0.294000
CG 24.880000
HG 1.683000
CD1 25.429000
HD1# 0.469000
CD2 19.921000
HD2# -0.193000
END_RES_DEF

RES_ID 733
RES_TYPE LYS
SPIN_SYSTEM_ID 19
HETEROGENEITY 100
N 118.568000
HN 8.563000
CA 60.125000
HA 3.679000
CB 32.588000
HB1 1.729000
HB2 1.360000
CG 24.880000
HG1 1.280000
CD 29.835000
HD1 1.585000
CE 41.960000
HE1 2.918000
END_RES_DEF

RES_ID 734
RES_TYPE SER
SPIN_SYSTEM_ID 20
HETEROGENEITY 100
N 113.157000
HN 7.540000
CA 61.227000
HA 4.281000
CB 63.879000
HB1 4.060000
END_RES_DEF

RES_ID 735
RES_TYPE ILE
SPIN_SYSTEM_ID 21
HETEROGENEITY 100
N 120.700000
HN 7.951000
CA 65.080000
HA 3.786000
CB 38.095000
HB 1.879000

CG1 28.733000
HG11 1.748000
HG12 1.052000
CG2 17.168000
HG2# 1.003000
CD1 13.863000
HD1# 0.619000
END_RES_DEF

RES_ID 736
RES_TYPE LEU
SPIN_SYSTEM_ID 22
HETEROGENEITY 100

N 119.880000
HN 8.841000
CA 58.473000
HA 4.090000
CB 41.950000
HB1 2.090000
HB2 1.703000
CG 27.330000
HG 1.759000
CD1 26.530000
HD1# 1.061000
CD2 23.776000
HD2# 0.977000
END_RES_DEF

RES_ID 737
RES_TYPE GLN
SPIN_SYSTEM_ID 23
HETEROGENEITY 100
N 117.256000
HN 8.505000
CA 59.020000
HA 4.032000
CB 28.182000
HB1 2.327000
HB2 2.263000
CG 34.240000
HG1 2.536000
HG2 2.461000
END_RES_DEF

RES_ID 738
RES_TYPE GLN
SPIN_SYSTEM_ID 24
HETEROGENEITY 100
N 118.896000
HN 8.033000
CA 59.574000
HA 4.196000
CB 29.835000
HB1 2.482000
HB2 2.469000
CG 35.342000
HG1 2.840000
HG2 2.467000
NE2 110.369000
HE21 7.022000
HE22 6.916000
END_RES_DEF

RES_ID 739
RES_TYPE VAL
SPIN_SYSTEM_ID 25
HETEROGENEITY 100
N 119.716000
HN 8.526000
CA 67.830000
HA 3.844000
CB 32.030000
HB 2.384000
CG1 23.330000
HG1# 1.183000
CG2 22.120000
HG2# 1.033000
END_RES_DEF

RES_ID 740
RES_TYPE LYS
SPIN_SYSTEM_ID 26
HETEROGENEITY 100
N 114.633000
HN 8.572000
CA 59.574000
HA 3.886000
CB 32.380000
HB1 1.873000
HG1 1.022000
HD1 1.520000
END_RES_DEF

RES_ID 741
RES_TYPE SER

SPIN_SYSTEM_ID 27
HETEROGENEITY 100
N 110.369000
HN 7.557000
CA 59.024000
HA 4.448000
CB 63.980000
HB1 4.004000
END_RES_DEF

RES_ID 742
RES_TYPE HIS
SPIN_SYSTEM_ID 28
HETEROGENEITY 100
N 125.619000
HN 7.536000
CA 58.473000
HA 3.967000
CB 32.588000
HB1 2.990000
HB2 2.799000
CD2 118.930000
HD2 4.978000
CE1 138.755000
HE1 7.522000
END_RES_DEF

RES_ID 743
RES_TYPE GLN
SPIN_SYSTEM_ID 29
HETEROGENEITY 100
N 128.571000
HN 8.543000
CA 59.125000
HA 4.209000
CB 29.834000
HB1 2.111000
CG 33.690000
HG1 2.390000
NE2 112.173000
HE21 7.581000
HE22 6.870000
END_RES_DEF

RES_ID 744
RES_TYPE SER
SPIN_SYSTEM_ID 30
HETEROGENEITY 100
N 119.060000
HN 11.668000
CA 60.125000
HA 4.838000
CB 63.980000
HB1 4.334000
HB2 3.926000
END_RES_DEF

RES_ID 745
RES_TYPE ALA
SPIN_SYSTEM_ID 31
HETEROGENEITY 100
N 117.584000
HN 7.868000
CA 53.510000
HA 4.396000
CB 20.470000
HB# 1.688000
END_RES_DEF

RES_ID 746
RES_TYPE TRP
SPIN_SYSTEM_ID 32
HETEROGENEITY 100
N 116.600000
HN 7.135000
CA 60.691000
HA 4.368000
CB 27.630000
HB1 3.594000
HB2 3.351000
CD1 128.843000
HD1 7.897000
NE1 110.861000
HE1 10.474000
CE3 122.234000
HE3 7.336000
CZ2 116.177000
H22 7.382000
CZ3 123.336000
H23 7.197000
CH2 126.089000
HH2 7.150000
END_RES_DEF

RES_ID 747

RES_TYPE PRO
SPIN_SYSTEM_ID 33
HETEROGENEITY 100
CA 64.531000
HA 3.756000
CB 29.835000
HB1 0.487000
HB2 -0.783000
CG 26.530000
HG1 0.233000
HG2 -0.931000
CD 50.212000
HD2 1.567000
HD1 2.177000
END_RES_DEF

RES_ID 748
RES_TYPE PHE
SPIN_SYSTEM_ID 34
HETEROGENEITY 100
N 113.321000
HN 7.585000
CA 55.719000
HA 4.930000
CB 39.202000
HB1 3.491000
HB2 2.532000
CD1 133.248000
HD1 7.099000
HE1 7.174000
HZ 7.296000
END_RES_DEF

RES_ID 749
RES_TYPE MET
SPIN_SYSTEM_ID 35
HETEROGENEITY 100
N 117.748000
HN 7.115000
CA 56.820000
HA 4.286000
CB 32.590000
HB1 2.233000
HB2 2.174000
CG 33.140000
HG1 2.851000
CE 17.168000
HE# 2.175000
END_RES_DEF

RES_ID 750
RES_TYPE GLU
SPIN_SYSTEM_ID 36
HETEROGENEITY 100
N 113.813000
HN 7.709000
CA 53.516000
HA 4.849000
CB 31.487000
HB1 2.091000
HB2 1.730000
CG 35.893000
HG1 2.164000
END_RES_DEF

RES_ID 751
RES_TYPE PRO
SPIN_SYSTEM_ID 37
HETEROGENEITY 100
CA 62.879000
HA 4.242000
CB 32.040000
HB1 2.328000
HB2 1.683000
CG 27.080000
HG1 2.126000
HG2 1.978000
CD 50.763000
HD1 3.670000
END_RES_DEF

RES_ID 752
RES_TYPE VAL
SPIN_SYSTEM_ID 38
HETEROGENEITY 100
N 124.450000
HN 8.124000
CA 63.430000
HA 3.553000
CB 32.580000
HB 1.145000
CG1 21.573000
HG1# 0.464000
CG2 21.573000
HG2# 0.169000

END_RES_DEF
RES_ID 753
RES_TYPE LYS
SPIN_SYSTEM_ID 39
HETEROGENEITY 100
N 129.883000
HN 9.045000
CA 56.310000
HA 4.370000
CB 32.880000
HB1 1.873000
HG1 1.435000
HD1 1.673000
HE1 2.985000
END_RES_DEF

RES_ID 754
RES_TYPE ARG
SPIN_SYSTEM_ID 40
HETEROGENEITY 100
N 120.208000
HN 8.054000
END_RES_DEF
RES_ID 755
RES_TYPE THR
SPIN_SYSTEM_ID 41
HETEROGENEITY 100
CA 63.430000
HA 4.038000
CB 68.380000
HB 4.293000
CG2 22.670000
HG2# 1.267000
END_RES_DEF

RES_ID 756
RES_TYPE GLU
SPIN_SYSTEM_ID 42
HETEROGENEITY 100
N 118.732000
HN 7.209000
CA 56.270000
HA 4.448000
CB 30.930000
HB1 2.174000
HB2 2.000000
CG 36.440000
HG1 2.292000
END_RES_DEF

RES_ID 757
RES_TYPE ALA
SPIN_SYSTEM_ID 43
HETEROGENEITY 100
N 122.504000
HN 7.379000
CA 50.220000
HA 4.937000
CB 19.370000
HB# 1.082000
END_RES_DEF

RES_ID 758
RES_TYPE PRO
SPIN_SYSTEM_ID 44
HETEROGENEITY 100
CA 65.080000
HA 4.496000
CB 31.487000
HB1 2.374000
HB2 2.027000
CG 27.632000
HG1 2.122000
HG2 2.038000
CD 50.212000
HD2 3.515000
HD1 3.717000
END_RES_DEF

RES_ID 759
RES_TYPE GLY
SPIN_SYSTEM_ID 45
HETEROGENEITY 100
END_RES_DEF
RES_ID 760
RES_TYPE TYR
SPIN_SYSTEM_ID 46
HETEROGENEITY 100
N 122.504000
HN 7.945000
CA 62.328000
HA 3.536000

CB 39.750000
HB1 2.689000
HB2 2.487000
CD1 133.799000
HD1 5.120000
CE1 118.379000
HE1 6.070000
END_RES_DEF

RES_ID 761
RES_TYPE TYR
SPIN_SYSTEM_ID 47
HETEROGENEITY 100
N 113.157000
HN 8.225000
CA 60.676000
HA 4.101000
CB 37.550000
HB1 3.189000
HB2 2.801000
CD1 134.901000
HD1 7.342000
CE1 118.930000
HE1 6.646000
END_RES_DEF

RES_ID 762
RES_TYPE GLU
SPIN_SYSTEM_ID 48
HETEROGENEITY 100
N 117.912000
HN 7.702000
CA 57.922000
HA 4.209000
CB 29.480000
HB1 2.086000
CG 37.545000
HG1 2.325000
HG2 2.265000
END_RES_DEF

RES_ID 763
RES_TYPE VAL
SPIN_SYSTEM_ID 49
HETEROGENEITY 100
N 115.453000
HN 7.135000
CA 63.430000
HA 4.077000
CB 33.690000
HB 2.015000
CG1 21.020000
HG1# 1.045000
CG2 21.574000
HG2# 0.991000
END_RES_DEF

RES_ID 764
RES_TYPE ILE
SPIN_SYSTEM_ID 50
HETEROGENEITY 100
N 122.832000
HN 7.947000
CA 57.920000
HA 3.916000
CB 34.240000
HB 1.205000
CG1 24.878000
HG11 0.798000
HG12 0.216000
CG2 16.617000
HG2# 0.380000
CD1 9.457000
HD1# 0.537000
END_RES_DEF

RES_ID 765
RES_TYPE ARG
SPIN_SYSTEM_ID 51
HETEROGENEITY 100
N 125.291000
HN 7.749000
CA 57.371000
HA 1.875000
CB 30.936000
HB1 1.388000
HB2 1.211000
CG 27.080000
HG1 1.319000
HG2 1.173000
CD 43.052000
HD1 2.971000
END_RES_DEF

RES_ID 766

RES_TYPE SER
SPIN_SYSTEM_ID 52
HETEROGENEITY 100
N 116.600000
HN 8.387000
CA 54.618000
HA 4.984000
CB 38.640000
HB1 3.034000
HB2 2.907000
END_RES_DEF

RES_ID 767
RES_TYPE PRO
SPIN_SYSTEM_ID 53
HETEROGENEITY 100

CA 63.429000
HA 4.083000
CB 32.588000
HB1 2.209000
CG 28.180000
HG1 2.177000
HG2 1.883000
CD 50.763000
HD2 3.390000
HD1 3.623000
END_RES_DEF

RES_ID 768
RES_TYPE MET
SPIN_SYSTEM_ID 54
HETEROGENEITY 100

N 119.060000
HN 8.430000
CA 54.067000
HA 4.935000
CB 31.487000
HB1 1.989000
HB2 1.353000
CG 30.930000
HG1 2.690000
CE 14.414000
HE# 1.929000
END_RES_DEF

RES_ID 769
RES_TYPE ASP
SPIN_SYSTEM_ID 55
HETEROGENEITY 100

N 119.060000
HN 7.365000
CA 53.516000
HA 4.745000
CB 44.154000
HB1 2.371000
END_RES_DEF

RES_ID 770
RES_TYPE LEU
SPIN_SYSTEM_ID 56
HETEROGENEITY 100

N 116.272000
HN 9.055000
CA 57.922000
HA 4.036000
CB 41.400000
HB1 2.095000
HB2 1.395000
CG 27.080000
HG 1.713000
CD1 27.080000
HD1# 0.940000
CD2 22.675000
HD2# 0.628000
END_RES_DEF

RES_ID 771
RES_TYPE LYS
SPIN_SYSTEM_ID 57
HETEROGENEITY 100

N 128.079000
HN 8.738000
CA 60.676000
HA 4.198000
CB 32.037000
HB1 2.330000
HB2 2.224000
CG 25.280000
HG1 1.483000
HG2 1.403000
CD 30.385000
HD1 1.793000
HD2 1.696000
CE 41.950000
HE1 2.965000

END_RES_DEF

RES_ID 772
RES_TYPE THR
SPIN_SYSTEM_ID 58
HETEROGENEITY 100

N 122.176000
HN 9.445000
CA 67.040000
HA 3.845000
CB 67.835000
HB 4.090000
CG2 22.124000
HG2# 1.058000
END_RES_DEF

RES_ID 773
RES_TYPE MET
SPIN_SYSTEM_ID 59
HETEROGENEITY 100

N 117.912000
HN 7.882000
CA 60.676000
HA 4.319000
CB 33.342000
HB1 2.093000
HB2 1.915000
CG 33.139000
HG1 2.621000
HG2 2.496000
CE 16.620000
HE# 1.241000
END_RES_DEF

RES_ID 774
RES_TYPE SER
SPIN_SYSTEM_ID 60
HETEROGENEITY 100

N 116.108000
HN 7.958000
CA 62.879000
HA 4.200000
CB 62.879000
HB1 4.368000
HB2 4.040000
END_RES_DEF

RES_ID 775
RES_TYPE GLU
SPIN_SYSTEM_ID 61
HETEROGENEITY 100

N 124.471000
HN 8.150000
CA 59.570000
HA 4.045000
CB 29.280000
HB1 2.246000
HB2 2.063000
CG 36.443000
HG1 2.345000
HG2 2.176000
END_RES_DEF

RES_ID 776
RES_TYPE ARG
SPIN_SYSTEM_ID 62
HETEROGENEITY 100

N 120.372000
HN 8.391000
CA 60.676000
HA 3.869000
CB 30.385000
HB1 2.047000
HB2 1.076000
CG 29.284000
HG1 1.722000
HG2 0.877000
CD 44.154000
HD1 2.578000
HD2 2.051000
END_RES_DEF

RES_ID 777
RES_TYPE LEU
SPIN_SYSTEM_ID 63
HETEROGENEITY 100

N 120.208000
HN 8.856000
CA 58.470000
HA 4.691000
CB 42.621000
HB1 2.295000
HB2 1.925000
CG 27.080000
HG 1.832000

CD1 25.429000
HD1# 1.067000
CD2 27.081000
HD2# 0.871000
END_RES_DEF

RES_ID 778
RES_TYPE LYS
SPIN_SYSTEM_ID 64
HETEROGENEITY 100

N 120.372000
HN 7.958000
CA 59.574000
HA 4.333000
CB 32.588000
HB1 2.055000
CG 24.878000
HG1 1.596000
CD 29.835000
HD1 1.804000
CE 41.951000
HE1 2.990000
END_RES_DEF

RES_ID 779
RES_TYPE ASN
SPIN_SYSTEM_ID 65
HETEROGENEITY 100

N 116.108000
HN 7.947000
CA 53.510000
HA 4.771000
CB 38.095000
HB1 3.019000
HB2 2.773000
ND2 112.665000
HD21 7.598000
HD22 6.969000
END_RES_DEF

RES_ID 780
RES_TYPE ARG
SPIN_SYSTEM_ID 66
HETEROGENEITY 100

N 114.141000
HN 8.158000
CA 56.821000
HA 4.405000
CB 25.429000
HB1 2.097000
HB2 2.022000
CG 27.632000
HG1 1.539000
HG2 1.534000
CD 43.050000
HD1 3.060000
HD2 3.024000
END_RES_DEF

RES_ID 781
RES_TYPE TYR
SPIN_SYSTEM_ID 67
HETEROGENEITY 100

N 116.764000
HN 8.222000
CA 60.125000
HA 4.064000
CB 40.850000
HB1 2.948000
HB2 2.055000
CD1 134.350000
HD1 6.285000
CE1 118.930000
HE1 6.709000
END_RES_DEF

RES_ID 782
RES_TYPE TYR
SPIN_SYSTEM_ID 68
HETEROGENEITY 100

N 114.633000
HN 8.014000
CA 57.920000
HA 4.528000
CB 36.443000
HB1 3.062000
HB2 2.907000
CD1 133.248000
HD1 7.175000
CE1 120.582000
HE1 7.286000
END_RES_DEF

RES_ID 783
RES_TYPE VAL

SPIN_SYSTEM_ID 69
HETEROGENEITY 100
N 115.780000
HN 7.698000
CA 62.330000
HA 4.083000
CB 31.500000
HB 2.321000
CG1 21.570000
HG1# 0.944000
CG2 18.820000
HG2# 0.823000
END_RES_DEF

RES_ID 784
RES_TYPE SER
SPIN_SYSTEM_ID 70
HETEROGENEITY 100

N 111.353000
HN 7.415000
CA 55.719000
HA 4.741000
CB 66.183000
HB1 4.200000
HB2 3.750000
END_RES_DEF

RES_ID 785
RES_TYPE LYS
SPIN_SYSTEM_ID 71
HETEROGENEITY 100

CA 59.030000
HA 4.021000
CB 31.590000
END_RES_DEF

RES_ID 786
RES_TYPE LYS
SPIN_SYSTEM_ID 72
HETEROGENEITY 100

N 120.208000
HN 8.244000
CA 59.720000
HA 4.062000
CB 30.385000
HB1 1.779000
CG 24.530000
CD 28.182000
HD1 1.680000
CE 41.670000
HE1 3.137000
HE2 3.045000
END_RES_DEF

RES_ID 787
RES_TYPE LEU
SPIN_SYSTEM_ID 73
HETEROGENEITY 100

N 118.732000
HN 7.422000
CA 57.922000
HA 4.213000
CB 43.603000
HB1 1.996000
HB2 1.891000
CG 27.632000
HG 1.794000
CD1 25.979000
HD1# 0.924000
CD2 23.776000
HD2# 0.895000
END_RES_DEF

RES_ID 788
RES_TYPE PHE
SPIN_SYSTEM_ID 74
HETEROGENEITY 100

N 118.732000
HN 6.928000
CA 60.676000
HA 3.763000
CB 39.750000
HB1 2.945000
HB2 2.381000
CD1 133.799000
HD1 6.400000
CE1 131.596000
HE1 6.928000
END_RES_DEF

RES_ID 789
RES_TYPE MET
SPIN_SYSTEM_ID 75
HETEROGENEITY 100
N 116.272000

HN 8.489000
CA 59.020000
HA 3.911000
CB 32.590000
HB1 2.318000
HB2 2.208000
CG 33.140000
HG1 2.942000
HG2 2.611000
CE 17.168000
HE# 2.027000
END_RES_DEF

RES_ID 790
RES_TYPE ALA
SPIN_SYSTEM_ID 76
HETEROGENEITY 100
N 119.716000
HN 8.000000
CA 55.170000
HA 4.084000
CB 18.270000
HB# 1.485000
END_RES_DEF

RES_ID 791
RES_TYPE ASP
SPIN_SYSTEM_ID 77
HETEROGENEITY 100
N 119.716000
HN 7.376000
CA 57.371000
HA 4.371000
CB 38.646000
HB1 2.730000
END_RES_DEF

RES_ID 792
RES_TYPE LEU
SPIN_SYSTEM_ID 78
HETEROGENEITY 100
N 119.550000
HN 7.363000
CA 57.922000
HA 3.398000
CB 40.299000
HB1 0.757000
HB2 0.442000
CG 27.632000
HG 0.707000
CD1 24.327000
HD1# 0.184000
CD2 25.979000
HD2# 0.061000
END_RES_DEF

RES_ID 793
RES_TYPE GLN
SPIN_SYSTEM_ID 79
HETEROGENEITY 100
N 114.141000
HN 8.069000
CA 59.024000
HA 3.804000
CB 28.733000
HB1 2.157000
HB2 2.097000
CG 35.342000
HG1 2.460000
HE2 111.353000
HE21 7.319000
HE22 7.222000
END_RES_DEF

RES_ID 794
RES_TYPE ARG
SPIN_SYSTEM_ID 80
HETEROGENEITY 100
N 118.568000
HN 7.382000
CA 58.473000
HA 4.078000
CB 29.835000
HB1 1.973000
HB2 1.886000
CG 27.080000
HG1 1.742000
CD 43.603000
HD1 3.390000
HD2 3.325000
END_RES_DEF

RES_ID 795
RES_TYPE VAL
SPIN_SYSTEM_ID 81

HETEROGENEITY 100
N 117.912000
HN 7.013000
CA 66.730000
HA 3.039000
CB 30.930000
HB 1.435000
CG1 22.124000
HG1# 0.479000
CG2 21.573000
HG2# 0.142000
END_RES_DEF

RES_ID 796
RES_TYPE PHE
SPIN_SYSTEM_ID 82
HETEROGENEITY 100
N 116.928000
HN 6.357000
CA 58.470000
HA 4.161000
CB 38.096000
HB1 3.090000
HB2 2.944000
CD1 132.147000
HD1 6.641000
CE1 131.596000
HE1 6.456000
CZ 129.393000
HZ 6.406000
END_RES_DEF

RES_ID 797
RES_TYPE THR
SPIN_SYSTEM_ID 83
HETEROGENEITY 100
N 115.289000
HN 9.047000
CA 66.734000
HA 3.838000
CB 68.380000
HB 4.210000
CG2 22.120000
HG2# 1.296000
END_RES_DEF

RES_ID 798
RES_TYPE ASN
SPIN_SYSTEM_ID 84
HETEROGENEITY 100
N 120.700000
HN 8.846000
CA 55.170000
HA 4.115000
CB 38.090000
HB1 2.985000
HB2 2.661000
END_RES_DEF

RES_ID 799
RES_TYPE CYS
SPIN_SYSTEM_ID 85
HETEROGENEITY 100
N 116.928000
HN 6.893000
CA 62.157000
HA 4.405000
CB 26.530000
HB1 3.304000
HB2 3.032000
END_RES_DEF

RES_ID 800
RES_TYPE LYS
SPIN_SYSTEM_ID 86
HETEROGENEITY 100
N 116.764000
HN 7.799000
CA 58.473000
HA 4.204000
CB 32.588000
HB1 1.743000
CG 25.429000
HG1 1.313000
HG2 0.138000
CD 29.835000
HD1 1.291000
CE 41.400000
HE1 2.486000
HE2 2.421000
END_RES_DEF

RES_ID 801
RES_TYPE GLU
SPIN_SYSTEM_ID 87

HETEROGENEITY 100
N 117.912000
HN 7.945000
CA 57.992000
HA 4.250000
CB 30.385000
HB1 2.172000
HB2 2.003000
CG 36.994000
HG1 2.407000
HG2 2.203000
END_RES_DEF

RES_ID 802
RES_TYPE TYR
SPIN_SYSTEM_ID 88
HETEROGENEITY 100
N 116.600000
HN 7.744000
CA 60.676000
HA 4.369000
CB 41.400000
HB1 2.929000
CD1 134.901000
HD1 6.989000
CE1 119.481000
HE1 6.823000
END_RES_DEF

RES_ID 803
RES_TYPE ASN
SPIN_SYSTEM_ID 89
HETEROGENEITY 100
N 115.944000
HN 8.241000
CA 51.864000
HA 5.024000
CB 40.849000
HB1 3.069000
HB2 2.907000
ND2 118.732000
HD21 8.316000
HD22 7.809000
END_RES_DEF

RES_ID 804
RES_TYPE ALA
SPIN_SYSTEM_ID 90
HETEROGENEITY 100
END_RES_DEF
RES_ID 805
RES_TYPE PRO
SPIN_SYSTEM_ID 91
HETEROGENEITY 100
CA 63.980000
HA 2.422000
HB1 1.949000
HG1 1.648000
HG2 1.558000
CD 50.762000
HD2 3.601000
HD1 3.706000
END_RES_DEF

RES_ID 806
RES_TYPE GLU
SPIN_SYSTEM_ID 92
HETEROGENEITY 100
N 112.993000
HN 8.246000
CA 56.820000
HA 4.185000
CB 28.733000
HB1 2.095000
HB2 1.973000
CG 36.270000
HG1 2.200000
END_RES_DEF

RES_ID 807
RES_TYPE SER
SPIN_SYSTEM_ID 93
HETEROGENEITY 100
N 115.780000
HN 8.112000
CA 58.473000
HA 4.406000
CB 66.183000
HB1 4.393000
HB2 4.157000
END_RES_DEF

RES_ID 808
RES_TYPE GLU

SPIN_SYSTEM_ID 94
HETEROGENEITY 100
N 123.488000
HN 9.061000
CA 59.574000
HA 4.232000
CB 29.835000
HB1 2.169000
CG 36.443000
HG1 2.528000
END_RES_DEF

RES_ID 809
RES_TYPE TYR
SPIN_SYSTEM_ID 95
HETEROGENEITY 100
N 116.436000
HN 8.072000
CA 60.120000
HA 3.834000
CB 37.550000
HB1 3.018000
HB2 2.738000
CD1 132.698000
HD1 6.891000
CE1 120.032000
HE1 7.011000
END_RES_DEF

RES_ID 810
RES_TYPE ASN
SPIN_SYSTEM_ID 96
HETEROGENEITY 100
N 119.880000
HN 7.356000
CA 61.777000
HA 3.819000
CB 40.300000
HB1 3.390000
HB2 2.500000
CD1 136.553000
HD1 7.094000
CE1 119.481000
HE1 7.000000
END_RES_DEF

RES_ID 811
RES_TYPE LYS
SPIN_SYSTEM_ID 97
HETEROGENEITY 100
N 118.076000
HN 8.072000
CA 60.676000
HA 4.204000
CB 32.588000
HB1 2.091000
CG 25.979000
HG1 1.819000
HG2 1.582000
CD 29.834000
HD1 1.813000
CE 41.963000
HE1 2.962000
END_RES_DEF

RES_ID 812
RES_TYPE CYS
SPIN_SYSTEM_ID 98
HETEROGENEITY 100
N 116.764000
HN 8.520000
CA 65.087000
HA 4.202000
CB 27.080000
HB1 3.396000
HB2 3.056000
END_RES_DEF

RES_ID 813
RES_TYPE ALA
SPIN_SYSTEM_ID 99
HETEROGENEITY 100
N 120.700000
HN 8.315000
CA 55.563000
HA 3.834000
CB 18.270000
HB# 1.597000
END_RES_DEF

RES_ID 814
RES_TYPE ASN
SPIN_SYSTEM_ID 100
HETEROGENEITY 100
N 115.453000

HN 8.068000
CA 56.270000
HA 4.329000
CB 38.646000
HB1 1.877000
HB2 2.834000
END_RES_DEF

RES_ID 815
RES_TYPE ILE
SPIN_SYSTEM_ID 101
HETEROGENEITY 100
N 119.880000
HN 7.912000
CA 65.080000
HA 3.646000
CB 39.197000
HB 1.924000
CG1 29.284000
HG11 1.882000
HG12 1.201000
CG2 17.718000
HG2# 1.017000
CD1 13.863000
HD1# 0.940000
END_RES_DEF

RES_ID 816
RES_TYPE LEU
SPIN_SYSTEM_ID 102
HETEROGENEITY 100
N 122.504000
HN 8.556000
CA 56.820000
HA 3.670000
CB 41.951000
HB1 1.405000
HB2 1.199000
CG 26.530000
HG 1.580000
CD1 24.327000
HD1# 0.701000
CD2 25.429000
HD2# 0.696000
END_RES_DEF

RES_ID 817
RES_TYPE GLU
SPIN_SYSTEM_ID 103
HETEROGENEITY 100
N 120.700000
HN 8.073000
CA 60.125000
HA 3.185000
CB 29.835000
HB1 1.720000
HB2 1.310000
CG 37.545000
HG1 2.001000
HG2 1.922000
END_RES_DEF

RES_ID 818
RES_TYPE LYS
SPIN_SYSTEM_ID 104
HETEROGENEITY 100
N 117.584000
HN 7.145000
CA 59.688000
HA 4.075000
CB 32.588000
HB1 1.929000
CG 25.644000
HG1 1.492000
CD 29.284000
HD1 1.681000
CE 41.963000
HE1 2.964000
END_RES_DEF

RES_ID 819
RES_TYPE PHE
SPIN_SYSTEM_ID 105
HETEROGENEITY 100
N 121.028000
HN 7.869000
CA 61.230000
HA 4.328000
CB 39.200000
HB1 3.133000
HB2 3.047000
CD1 133.800000
HD1 7.180000
END_RES_DEF

RES_ID 820
RES_TYPE PHE
SPIN_SYSTEM_ID 106
HETEROGENEITY 100
N 120.700000
HN 9.126000
CA 60.691000
HA 3.961000
CB 38.640000
HB1 3.289000
HB2 3.067000
CD1 133.248000
HD1 6.904000
CE1 132.698000
HE1 7.011000
END_RES_DEF

RES_ID 821
RES_TYPE PHE
SPIN_SYSTEM_ID 107
HETEROGENEITY 100
N 118.076000
HN 8.359000
CA 61.770000
HA 3.840000
CB 38.090000
HB1 3.064000
CD1 133.248000
HD1 7.175000
CE1 132.698000
HE1 7.294000
CZ 131.596000
HZ 7.430000
END_RES_DEF

RES_ID 822
RES_TYPE SER
SPIN_SYSTEM_ID 108
HETEROGENEITY 100
N 114.961000
HN 7.906000
CA 61.773000
HA 4.200000
CB 62.879000
HB1 4.007000
END_RES_DEF

RES_ID 823
RES_TYPE LYS
SPIN_SYSTEM_ID 109
HETEROGENEITY 100
N 120.864000
HN 7.938000
CA 56.820000
HA 4.008000
CB 31.487000
HB1 1.730000
HB2 1.567000
CG 23.226000
HG1 0.833000
CD 27.080000
HD1 1.403000
CE 42.501000
HE1 2.569000
HE2 2.422000
END_RES_DEF

RES_ID 824
RES_TYPE ILE
SPIN_SYSTEM_ID 110
HETEROGENEITY 100
N 116.928000
HN 8.101000
CA 64.530000
HA 3.818000
CB 36.990000
HB 1.746000
CG1 26.530000
HG11 1.140000
HG12 1.073000
CG2 18.820000
HG2# 0.654000
CD1 13.312000
HD1# 0.541000
END_RES_DEF

RES_ID 825
RES_TYPE LYS
SPIN_SYSTEM_ID 111
HETEROGENEITY 100
N 122.176000
HN 7.546000
CA 59.024000
HA 4.043000
CB 32.360000

HB1 1.879000
HB2 1.757000
CG 24.878000
HG1 1.390000
HG2 1.302000
CD 29.284000
HD1 1.633000
CE 41.400000
HE1 2.913000
END_RES_DEF

RES_ID 826
RES_TYPE GLU
SPIN_SYSTEM_ID 112
HETEROGENEITY 100
N 121.192000
HN 8.063000
CA 59.024000
HA 3.995000
CB 29.834000
HB1 2.058000
CG 36.050000
HG1 2.342000
HG2 2.205000
END_RES_DEF

RES_ID 827
RES_TYPE ALA
SPIN_SYSTEM_ID 113
HETEROGENEITY 100
N 117.748000
HN 7.620000
CA 52.410000
HA 4.291000
CB 19.920000
HB# 1.358000
END_RES_DEF

RES_ID 828
RES_TYPE GLY
SPIN_SYSTEM_ID 114
HETEROGENEITY 100
N 126.767000
HN 7.744000
CA 45.902000
HA1 4.019000
HA2 3.935000
END_RES_DEF

RES_ID 829
RES_TYPE LEU
SPIN_SYSTEM_ID 115
HETEROGENEITY 100
N 117.912000
HN 7.742000
CA 55.719000
HA 4.215000
CB 43.052000
HB1 1.562000
CG 27.632000
HG 1.536000
CD1 23.776000
HD1# 0.711000
END_RES_DEF

RES_ID 830
RES_TYPE ILE
SPIN_SYSTEM_ID 116
HETEROGENEITY 100
N 115.453000
HN 7.458000
CA 60.676000
HA 4.232000
CB 39.748000
HB 1.810000
CG1 27.080000
HG11 1.314000
HG12 0.918000
CG2 17.718000
HG2# 0.815000
CD1 13.312000
HD1# 0.794000
END_RES_DEF

RES_ID 831
RES_TYPE ASP
SPIN_SYSTEM_ID 117
HETEROGENEITY 100
N 123.488000
HN 8.270000
CA 54.620000
HA 4.571000
CB 41.400000
HB1 2.693000
HB2 2.540000

END_RES_DEF
RES_ID 832
RES_TYPE LYS
SPIN_SYSTEM_ID 118
HETEROGENEITY 100
N 125.450000
HN 7.774000
CA 57.720000
HA 4.082000
CB 33.410000
END_RES_DEF

Unambiguous NOE-derived Inter-proton Distance Restraints

1

3

7

ASSI (3711)
((segid "BRD " and resid 74 and name HN))
((segid "BRD " and resid 74 and name HN))
2 500 1 600 1 600 peak 3711 weight
0 110008:01 volume 0 731258:03 pval
7 994 pval2 4.004

ASSI (3714)
((segid "BRD " and resid 118 and name HN))
((segid "BRD " and resid 118 and name HN))
2 500 2 100 2 100 peak 3714 weight
0 110008:01 volume 0 308308:03 pval
4 689

ASSI (3715)
((segid "BRD " and resid 54 and name HN))
((segid "BRD " and resid 54 and name HN))
2 500 2 100 2 100 peak 3715 weight
0 110008:01 volume 0 304328:03 pval
5 546

ASSI (3771)
((segid "BRD " and resid 54 and name HN))
((segid "BRD " and resid 54 and name HN))
2 500 2 100 2 100 peak 3771 weight
0 110008:01 volume 0 125085:03 pval
2 596

ASSI (3781)
((segid "BRD " and resid 54 and name HN))
((segid "BRD " and resid 54 and name HN))
2 500 2 100 2 100 peak 3781 weight
0 110008:01 volume 0 326685:02 pval
1 960

ASSI (3791)
((segid "BRD " and resid 54 and name HN))
((segid "BRD " and resid 54 and name HN))
2 500 2 100 2 100 peak 3791 weight
0 110008:01 volume 0 184058:03 pval
4 900

ASSI (3801)
((segid "BRD " and resid 42 and name HN))
((segid "BRD " and resid 42 and name HN))
2 500 2 000 2 000 peak 3801 weight
0 110008:01 volume 0 369648:03 pval
4 467

ASSI (3811)
((segid "BRD " and resid 72 and name HN))
((segid "BRD " and resid 72 and name HN))
2 500 2 200 2 200 peak 3811 weight
0 110008:01 volume 0 244738:03 pval
4 660

ASSI (3821)
((segid "BRD " and resid 72 and name HN))
((segid "BRD " and resid 72 and name HN))
2 500 2 200 2 200 peak 3821 weight
0 110008:01 volume 0 748958:02 pval
4 033

ASSI (3831)
((segid "BRD " and resid 41 and name HN))
((segid "BRD " and resid 41 and name HN))
2 500 1 400 1 400 peak 3831 weight
0 110008:01 volume 0 821458:03 pval
4 462

ASSI (3841)
((segid "BRD " and resid 45 and name HN))
((segid "BRD " and resid 45 and name HN))
2 500 2 400 2 400 peak 3841 weight
0 110008:01 volume 0 222278:03 pval
4 476

ASSI (3851)
((segid "BRD " and resid 60 and name HN))
((segid "BRD " and resid 60 and name HN))
2 500 1 400 1 400 peak 3851 weight
0 110008:01 volume 0 107918:04 pval
4 408

ASSI (3861)
((segid "BRD " and resid 60 and name HN))
((segid "BRD " and resid 60 and name HN))
2 500 1 400 1 400 peak 3861 weight
0 110008:01 volume 0 100998:04 pval
4 467

ASSI (3891)
((segid "BRD " and resid 40 and name HN))
((segid "BRD " and resid 40 and name HN))
2 500 1 700 1 700 peak 3891 weight
0 110008:01 volume 0 652128:03 pval
4 975

ASSI (3901)
((segid "BRD " and resid 59 and name HN))
((segid "BRD " and resid 59 and name HN))
2 500 2 400 2 400 peak 3901 weight
0 110008:01 volume 0 187558:03 pval
4 893

ASSI (3921)
((segid "BRD " and resid 7 and name HN))
((segid "BRD " and resid 7 and name HN))
2 500 1 700 1 700 peak 3921 weight
0 110008:01 volume 0 431668:03 pval
4 968

ASSI (3931)
((segid "BRD " and resid 9 and name HN))
((segid "BRD " and resid 9 and name HN))
2 500 1 700 1 700 peak 3931 weight
0 110008:01 volume 0 553468:03 pval
4 938

ASSI (3941)
((segid "BRD " and resid 13 and name HN))
((segid "BRD " and resid 13 and name HN))
2 500 2 600 2 600 peak 3941 weight
0 110008:01 volume 0 182058:03 pval
5 299

ASSI (3951)
((segid "BRD " and resid 16 and name HN))
((segid "BRD " and resid 16 and name HN))
2 500 2 700 2 700 peak 3951 weight
0 110008:01 volume 0 137228:03 pval
3 618

ASSI (3961)
((segid "BRD " and resid 15 and name HN))
((segid "BRD " and resid 15 and name HN))
2 500 1 600 1 600 peak 3961 weight
0 110008:01 volume 0 740928:03 pval
3 431

ASSI (3971)
((segid "BRD " and resid 17 and name HN))
((segid "BRD " and resid 17 and name HN))
2 500 1 600 1 600 peak 3971 weight
0 110008:01 volume 0 424698:03 pval
4 936

ASSI (3981)
((segid "BRD " and resid 18 and name HN))
((segid "BRD " and resid 18 and name HN))
2 500 2 200 2 200 peak 3981 weight
0 110008:01 volume 0 245818:03 pval
3 878

ASSI (4001)
((segid "BRD " and resid 18 and name HN))
((segid "BRD " and resid 18 and name HN))
2 500 2 000 2 000 peak 4001 weight
0 110008:01 volume 0 364628:03 pval
4 884

ASSI (4011)
((segid "BRD " and resid 18 and name HN))
((segid "BRD " and resid 18 and name HN))
2 500 2 000 2 000 peak 4011 weight
0 110008:01 volume 0 364628:03 pval
4 884

[illegible]

[illegible]

[illegible]

21

((segid "BTD" * and readid 41 and name H0231))	2.400	1.400	1.400 peak 10571 weight	0.10000E+01 volume	0.10119E+04 ppm1	7.975 ppm2	3.105
ASST [10281]							
((segid "BTD" * and readid 76 and name HN1))	3.000	2.200	2.200 peak 10581 weight	0.10000E+01 volume	0.24476E+03 ppm1	7.974 ppm2	3.301
ASST [10291]							
((segid "BTD" * and readid 55 and name HN1))	4.100	4.000	1.400 peak 10591 weight	0.10000E+01 volume	0.42390E+02 ppm1	7.972 ppm2	10.042
ASST [10291]							
((segid "BTD" * and readid 54 and name HN1))	3.700	3.400	1.800 peak 10591 weight	0.10000E+01 volume	0.69879E+02 ppm1	9.674 ppm2	4.100
ASST [10441]							
((segid "BTD" * and readid 82 and name HN1))	4.200	4.200	1.300 peak 10611 weight	0.10000E+01 volume	0.33240E+02 ppm1	6.981 ppm2	2.403
ASST [10441]							
((segid "BTD" * and readid 82 and name HN1))	4.300	4.300	1.200 peak 10651 weight	0.10000E+01 volume	0.31942E+02 ppm1	6.981 ppm2	3.220
ASST [10441]							
((segid "BTD" * and readid 82 and name HN1))	4.100	4.100	1.400 peak 10651 weight	0.10000E+01 volume	0.41756E+02 ppm1	6.981 ppm2	2.302
ASST [10721]							
((segid "BTD" * and readid 81 and name HN1))	3.800	3.800	1.600 peak 10711 weight	0.10000E+01 volume	0.54085E+02 ppm1	7.641 ppm2	3.210
ASST [10731]							
((segid "BTD" * and readid 80 and name HN1))	4.400	4.400	1.100 peak 10751 weight	0.10000E+01 volume	0.26321E+02 ppm1	8.005 ppm2	3.222
ASST [10771]							
((segid "BTD" * and readid 80 and name HN1))	3.700	3.400	1.800 peak 10771 weight	0.10000E+01 volume	0.71103E+02 ppm1	8.006 ppm2	2.049
ASST [10841]							
((segid "BTD" * and readid 85 and name HN1))	3.800	3.100	2.000 peak 10841 weight	0.10000E+01 volume	0.10980E+03 ppm1	8.681 ppm2	2.096
ASST [10881]							
((segid "BTD" * and readid 85 and name HN1))	3.800	3.800	1.600 peak 10881 weight	0.10000E+01 volume	0.36640E+02 ppm1	7.515 ppm2	2.208
ASST [10901]							
((segid "BTD" * and readid 81 and name H0241))	4.100	4.100	1.400 peak 10891 weight	0.10000E+01 volume	0.42361E+02 ppm1	7.532 ppm2	0.765
ASST [10921]							
((segid "BTD" * and readid 86 and name HN1))	3.800	3.400	1.700 peak 10921 weight	0.10000E+01 volume	0.59408E+02 ppm1	8.403 ppm2	2.779
OR [10921]							
((segid "BTD" * and readid 86 and name HN1))	3.800	3.400	1.700 peak 10921 weight	0.10000E+01 volume	0.59561E+02 ppm1	8.433 ppm2	2.577
ASST [10941]							
((segid "BTD" * and readid 86 and name HN1))	3.800	3.400	1.700 peak 10941 weight	0.10000E+01 volume	0.93245E+02 ppm1	8.422 ppm2	2.210
ASST [11001]							
((segid "BTD" * and readid 87 and name HN1))	3.400	3.400	1.700 peak 11001 weight	0.10000E+01 volume	0.61476E+02 ppm1	8.570 ppm2	3.146
ASST [11021]							
((segid "BTD" * and readid 87 and name HN1))	4.500	4.500	1.000 peak 11021 weight	0.10000E+01 volume	0.22088E+02 ppm1	8.571 ppm2	0.780
ASST [11031]							
((segid "BTD" * and readid 88 and name HN1))	3.600	3.200	1.900 peak 11031 weight	0.10000E+01 volume	0.90228E+02 ppm1	8.356 ppm2	3.166
ASST [11041]							
((segid "BTD" * and readid 88 and name HN1))	4.000	4.000	0.900 peak 11051 weight	0.10000E+01 volume	0.19886E+02 ppm1	8.356 ppm2	3.018
ASST [11161]							
((segid "BTD" * and readid 91 and name HN1))	3.700	3.400	1.600 peak 11161 weight	0.10000E+01 volume	0.78154E+02 ppm1	8.714 ppm2	4.410
ASST [11171]							
((segid "BTD" * and readid 93 and name HN1))	3.700	3.700	2.200 peak 11171 weight	0.10000E+01 volume	0.19982E+03 ppm1	8.714 ppm2	4.004
ASST [11191]							
((segid "BTD" * and readid 10 and name HN1))	2.500	1.600	1.400 peak 9851 weight	0.10000E+01 volume	0.73405E+03 ppm1	8.469 ppm2	1.866
ASST [9971]							
((segid "BTD" * and readid 72 and name HN1))	2.200	2.200	2.200 peak 9971 weight	0.10000E+01 volume	0.46134E+02 ppm1	8.468 ppm2	1.379
ASST [9981]							
((segid "BTD" * and readid 14 and name HN1))	4.100						

1000000.01 volume 0.139218-02 ppm1

((segid "BPD" - and resid 24 and name H21)) ASST [11201] 4.400 4.400 1.100 peak 1191 weight 0.10000E-01 volume 0.46154E-02 ppm1	12.276 ppm2	3.192
((segid "BPD" - and resid 30 and name H1)) ASST [11201] 4.400 4.400 1.100 peak 1201 weight 0.10000E-01 volume 0.437218-02 ppm1	8.649 ppm2	4.285
((segid "BPD" - and resid 24 and name H21)) ASST [11201] 2.700 2.700 2.200 peak 1191 weight 0.10000E-01 volume 0.139218-02 ppm1	8.649 ppm2	2.519
((segid "BPD" - and resid 30 and name H1)) ASST [11201] 3.600 3.600 1.900 peak 1191 weight 0.10000E-01 volume 0.38443E-02 ppm1	8.649 ppm2	2.519
((segid "BPD" - and resid 31 and name H1)) ASST [11201] 3.600 3.600 1.900 peak 1191 weight 0.10000E-01 volume 0.14273E-03 ppm1	8.981 ppm2	7.515
((segid "BPD" - and resid 31 and name H1)) ASST [11201] 3.600 3.600 1.900 peak 1191 weight 0.10000E-01 volume 0.11369E-03 ppm1	8.981 ppm2	2.547
((segid "BPD" - and resid 31 and name H1)) ASST [11201] 3.600 3.600 1.900 peak 1191 weight 0.10000E-01 volume 0.44466E-02 ppm1	8.981 ppm2	1.678
((segid "BPD" - and resid 31 and name H1)) ASST [11201] 3.600 3.600 1.900 peak 1191 weight 0.10000E-01 volume 0.20202E-00 ppm1	8.981 ppm2	2.195
((segid "BPD" - and resid 31 and name H1)) ASST [11201] 3.600 3.600 1.900 peak 1191 weight 0.10000E-01 volume 0.28750E-02 ppm1	8.981 ppm2	1.728
((segid "BPD" - and resid 31 and name H1)) ASST [11201] 3.600 3.600 1.900 peak 1191 weight 0.10000E-01 volume 0.12771E-03 ppm1	8.981 ppm2	1.275
((segid "BPD" - and resid 31 and name H1)) ASST [11201] 3.600 3.600 1.900 peak 1191 weight 0.10000E-01 volume 0.11633E-03 ppm1	8.981 ppm2	1.969
((segid "BPD" - and resid 31 and name H1)) ASST [11201] 3.600 3.600 1.900 peak 1191 weight 0.10000E-01 volume 0.47661E-02 ppm1	8.981 ppm2	1.558
((segid "BPD" - and resid 31 and name H1)) ASST [11201] 3.600 3.600 1.900 peak 1191 weight 0.10000E-01 volume 0.26420E-02 ppm1	8.981 ppm2	1.163
((segid "BPD" - and resid 31 and name H1)) ASST [11201] 3.600 3.600 1.900 peak 1191 weight 0.10000E-01 volume 0.76041E-02 ppm1	8.981 ppm2	2.346
((segid "BPD" - and resid 31 and name H1)) ASST [11201] 3.600 3.600 1.900 peak 1191 weight 0.10000E-01 volume 0.17261E-02 ppm1	8.981 ppm2	1.544
((segid "BPD" - and resid 31 and name H1)) ASST [11201] 3.600 3.600 1.900 peak 1191 weight 0.10000E-01 volume 0.16530E-03 ppm1	8.981 ppm2	1.277
((segid "BPD" - and resid 31 and name H1)) ASST [11201] 3.600 3.600 1.900 peak 1191 weight 0.10000E-01 volume 0.17496E-03 ppm1	8.981 ppm2	1.156
((segid "BPD" - and resid 31 and name H1)) ASST [11201] 3.600 3.600 1.900 peak 1191 weight 0.10000E-01 volume 0.33541E-02 ppm1	8.981 ppm2	2.861
((segid "BPD" - and resid 31 and name H1)) ASST [11201] 3.600 3.600 1.900 peak 1191 weight 0.10000E-01 volume 0.60519E-02 ppm1	8.981 ppm2	1.700
((segid "BPD" - and resid 31 and name H1)) ASST [11201] 3.600 3.600 1.900 peak 1191 weight 0.10000E-01 volume 0.90941E-02 ppm1	7.762 ppm2	1.787
((segid "BPD" - and resid 31 and name H1)) ASST [11201] 3.600 3.600 1.900 peak 1191 weight 0.10000E-01 volume 0.53605E-02 ppm1	9.004 ppm2	2.820
((segid "BPD" - and resid 31 and name H1)) ASST [11201] 3.600 3.600 1.900 peak 1191 weight 0.10000E-01 volume 0.21402E-03 ppm1	7.420 ppm2	2.491
((segid "BPD" - and resid 31 and name H1)) ASST [11201] 3.600 3.600 1.900 peak 1191 weight 0.10000E-01 volume 0.25898E-03 ppm1	7.421 ppm2	2.266

[illegible]

[illegible]

27

29

ASST (4502)
((segid "BPD" and resid 98 and name HA))
((segid "BPD" and resid 99 and name HB))
2.700 1.800 1.800 peak 6502 weight 0.11000E+01 volume 0.13206E+03 ppm1 4.804 ppm2 3.660
ASST (4512)
((segid "BPD" and resid 32 and name HA))
((segid "BPD" and resid 33 and name HB))
1.800 1.800 peak 6512 weight 0.11000E+01 volume 0.22946E+03 ppm1 4.953 ppm2 3.965
ASST (4522)
((segid "BPD" and resid 32 and name HA))
((segid "BPD" and resid 33 and name HB))
2.700 1.800 1.800 peak 6522 weight 0.11000E+01 volume 0.20647E+03 ppm1 4.954 ppm2 4.206
ASST (4532)
((segid "BPD" and resid 32 and name HA))
((segid "BPD" and resid 33 and name HB))
2.700 1.800 1.800 peak 6532 weight 0.11000E+01 volume 0.21807E+03 ppm1 4.951 ppm2 2.635
ASST (4542)
((segid "BPD" and resid 32 and name HA))
((segid "BPD" and resid 33 and name HB))
2.700 1.800 1.800 peak 6542 weight 0.11000E+01 volume 0.20893E+03 ppm1 2.784 ppm2 4.687
ASST (4552)
((segid "BPD" and resid 32 and name HA))
((segid "BPD" and resid 33 and name HB))
2.700 1.800 1.800 peak 6552 weight 0.11000E+01 volume 0.24090E+03 ppm1 5.000 ppm2 1.323
ASST (4562)
((segid "BPD" and resid 32 and name HA))
((segid "BPD" and resid 33 and name HB))
2.700 1.800 1.800 peak 6562 weight 0.11000E+01 volume 0.31261E+03 ppm1 2.289 ppm2 1.320
ASST (4572)
((segid "BPD" and resid 32 and name HA))
((segid "BPD" and resid 33 and name HB))
2.700 1.800 1.800 peak 6572 weight 0.11000E+01 volume 0.39478E+03 ppm1 5.547 ppm2 4.127
ASST (4582)
((segid "BPD" and resid 32 and name HA))
((segid "BPD" and resid 33 and name HB))
2.700 1.800 1.800 peak 6582 weight 0.11000E+01 volume 0.20471E+03 ppm1 1.700 ppm2 4.135
ASST (4592)
((segid "BPD" and resid 32 and name HA))
((segid "BPD" and resid 33 and name HB))
2.700 1.800 1.800 peak 6592 weight 0.11000E+01 volume 0.27108E+03 ppm1 1.697 ppm2 3.295
ASST (4602)
((segid "BPD" and resid 32 and name HA))
((segid "BPD" and resid 33 and name HB))
2.700 1.800 1.800 peak 6602 weight 0.11000E+01 volume 0.14513E+03 ppm1 4.658 ppm2 2.774
ASST (4612)
((segid "BPD" and resid 32 and name HA))
((segid "BPD" and resid 33 and name HB))
2.700 1.800 1.800 peak 6612 weight 0.11000E+01 volume 0.31689E+03 ppm1 1.994 ppm2 1.750
ASST (4622)
((segid "BPD" and resid 32 and name HA))
((segid "BPD" and resid 33 and name HB))
2.700 1.800 1.800 peak 6622 weight 0.11000E+01 volume 0.13650E+03 ppm1 1.700 ppm2 4.137
ASST (4632)
((segid "BPD" and resid 32 and name HA))
((segid "BPD" and resid 33 and name HB))
2.700 1.800 1.800 peak 6632 weight 0.11000E+01 volume 0.21235E+03 ppm1 1.995 ppm2 1.323
ASST (4642)
((segid "BPD" and resid 32 and name HA))
((segid "BPD" and resid 33 and name HB))
2.700 1.800 1.800 peak 6642 weight 0.11000E+01 volume 0.27725E+03 ppm1 1.446 ppm2 1.324
ASST (4652)
((segid "BPD" and resid 32 and name HA))
((segid "BPD" and resid 33 and name HB))
2.700 1.800 1.800 peak 6652 weight 0.11000E+01 volume 0.16697E+03 ppm1 1.644 ppm2 0.775
ASST (4662)
((segid "BPD" and resid 32 and name HA))
((segid "BPD" and resid 33 and name HB))
2.700 1.800 1.800 peak 6662 weight 0.11000E+01 volume 0.17527E+03 ppm1 1.751 ppm2 4.170
ASST (4672)
((segid "BPD" and resid 32 and name HA))
((segid "BPD" and resid 33 and name HB))
2.700 1.800 1.800 peak 6672 weight 0.11000E+01 volume 0.74974E+03 ppm1 0.806 ppm2 1.715
ASST (4682)
((segid "BPD" and resid 32 and name HA))
((segid "BPD" and resid 33 and name HB))
2.700 1.800 1.800 peak 6682 weight 0.11000E+01 volume 0.12930E+03 ppm1 4.852 ppm2 1.897

35

[illegible]


```

ASSI [ 10152 ]
(( segid "brd" * and read 66 and name H81 ))
(( segid "brd" * and read 98 and name H81 ))
2.700 1.800 1.600 peak 30152 weight 0.11000E+01 volume 0.21345E+03 ppm1 2.338 ppm2 7.603 1.599 ppm2 1.444

ASSI [ 10153 ]
(( segid "brd" * and read 86 and name H81 ))
(( segid "brd" * and read 86 and name H81 ))
2.400 2.400 peak 30153 weight 0.11000E+01 volume 0.98050E+02 ppm1 3.000 ppm2 4.808 2.291 ppm2 1.539

ASSI [ 10154 ]
(( segid "brd" * and read 86 and name H81 ))
(( segid "brd" * and read 86 and name H81 ))
2.200 1.200 1.200 peak 30154 weight 0.11000E+01 volume 0.44118E+03 ppm1 3.079 ppm2 1.496 2.190 ppm2 4.752

ASSI [ 10155 ]
(( segid "brd" * and read 86 and name H81 ))
(( segid "brd" * and read 86 and name H81 ))
2.200 1.200 1.200 peak 30155 weight 0.11000E+01 volume 0.14017E+03 ppm1 3.079 ppm2 1.496 2.190 ppm2 4.752

ASSI [ 10156 ]
(( segid "brd" * and read 109 and name H81 ))
(( segid "brd" * and read 109 and name H81 ))
2.100 2.100 peak 30156 weight 0.11000E+01 volume 0.12187E+03 ppm1 3.176 ppm2 4.639 2.190 ppm2 4.752

ASSI [ 10157 ]
(( segid "brd" * and read 109 and name H81 ))
(( segid "brd" * and read 109 and name H81 ))
2.100 2.100 peak 30157 weight 0.11000E+01 volume 0.17943E+04 ppm1 1.994 ppm2 4.639 2.190 ppm2 4.752

ASSI [ 10158 ]
(( segid "brd" * and read 109 and name H81 ))
(( segid "brd" * and read 109 and name H81 ))
2.100 2.100 peak 30158 weight 0.11000E+01 volume 0.44758E+03 ppm1 2.338 ppm2 4.575 2.190 ppm2 4.752

ASSI [ 10159 ]
(( segid "brd" * and read 109 and name H81 ))
(( segid "brd" * and read 109 and name H81 ))
2.100 2.100 peak 30159 weight 0.11000E+01 volume 0.21060E+03 ppm1 2.179 ppm2 4.575 2.190 ppm2 4.752

ASSI [ 10160 ]
(( segid "brd" * and read 109 and name H81 ))
(( segid "brd" * and read 109 and name H81 ))
2.100 2.100 peak 30160 weight 0.11000E+01 volume 0.42105E+03 ppm1 2.113 ppm2 4.800 2.190 ppm2 4.752

ASSI [ 10161 ]
(( segid "brd" * and read 109 and name H81 ))
(( segid "brd" * and read 109 and name H81 ))
2.100 2.100 peak 30161 weight 0.11000E+01 volume 0.32351E+04 ppm1 2.289 ppm2 4.671 2.190 ppm2 4.752

ASSI [ 10162 ]
(( segid "brd" * and read 111 and name H81 ))
(( segid "brd" * and read 111 and name H81 ))
2.100 2.100 peak 30162 weight 0.11000E+01 volume 0.72638E+03 ppm1 3.520 ppm2 4.656 2.190 ppm2 4.752

ASSI [ 10163 ]
(( segid "brd" * and read 111 and name H81 ))
(( segid "brd" * and read 111 and name H81 ))
2.100 2.100 peak 30163 weight 0.11000E+01 volume 0.50216E+03 ppm1 2.287 ppm2 3.744 2.190 ppm2 4.752

ASSI [ 10164 ]
(( segid "brd" * and read 111 and name H81 ))
(( segid "brd" * and read 111 and name H81 ))
2.100 2.100 peak 30164 weight 0.11000E+01 volume 0.79378E+03 ppm1 2.387 ppm2 3.744 2.190 ppm2 4.752

ASSI [ 10165 ]
(( segid "brd" * and read 111 and name H81 ))
(( segid "brd" * and read 111 and name H81 ))
2.100 2.100 peak 30165 weight 0.11000E+01 volume 0.15518E+04 ppm1 2.386 ppm2 3.452 2.190 ppm2 4.752

ASSI [ 10166 ]
(( segid "brd" * and read 111 and name H81 ))
(( segid "brd" * and read 111 and name H81 ))
2.100 2.100 peak 30166 weight 0.11000E+01 volume 0.10163E+04 ppm1 1.154 ppm2 1.309 2.190 ppm2 4.752

ASSI [ 10167 ]
(( segid "brd" * and read 111 and name H81 ))
(( segid "brd" * and read 111 and name H81 ))
2.100 2.100 peak 30167 weight 0.11000E+01 volume 0.30439E+03 ppm1 3.029 ppm2 2.351 2.190 ppm2 4.752

ASSI [ 10168 ]
(( segid "brd" * and read 111 and name H81 ))
(( segid "brd" * and read 111 and name H81 ))
2.100 2.100 peak 30168 weight 0.11000E+01 volume 0.22163E+03 ppm1 2.191 ppm2 1.495 2.190 ppm2 4.752

ASSI [ 10169 ]
(( segid "brd" * and read 111 and name H81 ))
(( segid "brd" * and read 111 and name H81 ))
2.100 2.100 peak 30169 weight 0.11000E+01 volume 0.10809E+03 ppm1 2.683 ppm2 1.580 2.190 ppm2 4.752

ASSI [ 10170 ]
(( segid "brd" * and read 111 and name H81 ))
(( segid "brd" * and read 111 and name H81 ))
2.100 2.100 peak 30170 weight 0.11000E+01 volume 0.14817E+03 ppm1 2.586 ppm2 5.380 2.190 ppm2 4.752

ASSI [ 10171 ]
(( segid "brd" * and read 111 and name H81 ))
(( segid "brd" * and read 111 and name H81 ))
2.100 2.100 peak 30171 weight 0.11000E+01 volume 0.21496E+03 ppm1 2.140 ppm2 1.222 2.190 ppm2 4.752

ASSI [ 10172 ]
(( segid "brd" * and read 111 and name H81 ))
(( segid "brd" * and read 111 and name H81 ))
2.100 2.100 peak 30172 weight 0.11000E+01 volume 0.62220E+02 ppm1 1.599 ppm2 0.677 2.190 ppm2 4.752

```


ASST [13092] 3.500 3.100 2.000 peak 13092 weight 0.10000E+01 volume 0.44548E+02 ppm1 2.464 3.177 ppm2 3.499 4.360 ppm2

ASST [13092]	3.500	3.100	2.000 peak 13092 weight	0.10000E+01 volume	0.44548E+02 ppm1	2.464	3.177 ppm2	3.499	4.360 ppm2
((segid "BPD" and resid 59 and name HB2))									
((segid "BPD" and resid 54 and name HB1))									
ASST [13102]	3.500	3.100	2.000 peak 13102 weight	0.10000E+01 volume	0.51668E+02 ppm1	1.075	3.288 ppm2	3.464	2.091 ppm2
((segid "BPD" and resid 71 and name HB1))									
ASST [13112]	3.500	3.100	2.000 peak 13112 weight	0.10000E+01 volume	0.10760E+03 ppm1	5.142	2.486 ppm2	5.362	1.402 ppm2
((segid "BPD" and resid 68 and name HB1))									
ASST [13122]	3.500	3.100	2.000 peak 13122 weight	0.10000E+01 volume	0.13268E+03 ppm1	5.141	2.583 ppm2	5.362	1.402 ppm2
((segid "BPD" and resid 73 and name HB1))									
ASST [13132]	3.500	3.100	2.000 peak 13132 weight	0.10000E+01 volume	0.45934E+02 ppm1	0.790	3.275 ppm2	4.933	3.667 ppm2
((segid "BPD" and resid 36 and name HB1))									
ASST [13142]	3.500	3.100	2.000 peak 13142 weight	0.10000E+01 volume	0.86018E+02 ppm1	1.437	4.407 ppm2	2.136	4.459 ppm2
((segid "BPD" and resid 22 and name HB1))									
OR [13152]									
ASST [13162]	3.500	3.100	2.000 peak 13162 weight	0.10000E+01 volume	0.18778E+03 ppm1	1.145	1.548 ppm2	3.561	4.457 ppm2
((segid "BPD" and resid 56 and name HB1))									
ASST [13172]	3.500	3.100	2.000 peak 13172 weight	0.10000E+01 volume	0.12726E+03 ppm1	1.252	1.795 ppm2	2.218	5.000 ppm2
((segid "BPD" and resid 116 and name HB1))									
ASST [13182]	3.500	3.100	2.000 peak 13182 weight	0.10000E+01 volume	0.34390E+03 ppm1	2.516	1.648 ppm2	4.437	2.289 ppm2
((segid "BPD" and resid 25 and name HB1))									
ASST [13192]	3.500	3.100	2.000 peak 13192 weight	0.10000E+01 volume	0.10896E+03 ppm1	1.956	2.434 ppm2	3.318	2.338 ppm2
((segid "BPD" and resid 54 and name HB1))									
ASST [13202]	3.500	3.100	2.000 peak 13202 weight	0.10000E+01 volume	0.27127E+03 ppm1	1.417	2.634 ppm2	2.495	1.198 ppm2
((segid "BPD" and resid 49 and name HB1))									
ASST [13212]	3.500	3.100	2.000 peak 13212 weight	0.10000E+01 volume	0.37432E+02 ppm1	2.101	2.537 ppm2	1.435	4.555 ppm2
((segid "BPD" and resid 63 and name HB1))									
ASST [13222]	3.500	3.100	2.000 peak 13222 weight	0.10000E+01 volume	0.44471E+02 ppm1	3.662	5.396 ppm2	2.042	4.406 ppm2
((segid "BPD" and resid 19 and name HB1))									
ASST [13232]	3.500	3.100	2.000 peak 13232 weight	0.10000E+01 volume	0.20244E+03 ppm1	1.956	1.498 ppm2	2.181	4.411 ppm2
((segid "BPD" and resid 64 and name HB1))									
OR [13242]									
ASST [13252]	3.500	3.100	2.000 peak 13252 weight	0.10000E+01 volume	0.18294E+02 ppm1	1.488	4.951 ppm2	1.320	1.254 ppm2
((segid "BPD" and resid 49 and name HB1))									
ASST [13262]	3.500	3.100	2.000 peak 13262 weight	0.10000E+01 volume	0.26015E+02 ppm1	1.009	1.646 ppm2	1.278	1.949 ppm2
((segid "BPD" and resid 76 and name HB1))									
ASST [13272]	3.500	3.100	2.000 peak 13272 weight	0.10000E+01 volume	0.14558E+02 ppm1	2.508	4.656 ppm2	2.351	3.866 ppm2
((segid "BPD" and resid 80 and name HB1))									
ASST [13282]	3.500	3.100	2.000 peak 13282 weight	0.10000E+01 volume	0.92421E+02 ppm1	3.159	2.685 ppm2	2.467	1.057 ppm2
((segid "BPD" and resid 34 and name HB1))									
ASST [13292]	3.500	3.100	2.000 peak 13292 weight	0.10000E+01 volume	0.54015E+02 ppm1	4.483	2.636 ppm2	1.458	1.205 ppm2
((segid "BPD" and resid 67 and name HB1))									
ASST [13302]	3.500	3.100	2.000 peak 13302 weight	0.10000E+01 volume	0.15688E+02 ppm1	1.030	1.425 ppm2	1.075	2.515 ppm2
((segid "BPD" and resid 18 and name HB1))									
OR [13312]									
ASST [13322]	3.500	3.100	2.000 peak 13322 weight	0.10000E+01 volume	0.14355E+02 ppm1	0.880	1.425 ppm2	4.222	4.460 ppm2
((segid "BPD" and resid 12 and name HB1))									
ASST [13332]	3.500	3.100	2.000 peak 13332 weight	0.10000E+01 volume	0.11539E+03 ppm1	1.382	5.298 ppm2	2.986	5.446 ppm2
((segid "BPD" and resid 14 and name HB1))									
ASST [13342]	3.500	3.100	2.000 peak 13342 weight	0.10000E+01 volume	0.60436E+03 ppm1				
((segid "BPD" and resid 74 and name HB1))									

[illegible]

[illegible]

ASST [25432]	3.300	2.700	2.200 peak 24782 weight	0.10000E+01 volume	0.57850E+02 ppm1	1.855 ppm2	7.489	4.804 ppm2	5.444
((segid "BRD" and resid 19 and name H1))									
((segid "BRD" and resid 15 and name H1))									
ASST [25432]	2.400	1.400	1.400 peak 24832 weight	0.10000E+01 volume	0.17891E+03 ppm1	2.191 ppm2	7.469	4.804 ppm2	7.779
((segid "BRD" and resid 19 and name H1))									
ASST [25432]	2.400	2.300	2.300 peak 24842 weight	0.10000E+01 volume	0.74418E+03 ppm1	2.191 ppm2	1.454	4.013 ppm2	4.933
((segid "BRD" and resid 19 and name H1))									
ASST [25432]	2.600	1.700	1.700 peak 24852 weight	0.10000E+01 volume	0.24553E+03 ppm1	3.124 ppm2	1.888	4.015 ppm2	4.533
((segid "BRD" and resid 23 and name H2))									
ASST [25432]	2.500	1.800	1.800 peak 24892 weight	0.10000E+01 volume	0.29588E+03 ppm1	3.068 ppm2	1.888	3.620 ppm2	2.206
((segid "BRD" and resid 21 and name H2))									
ASST [25432]	2.400	1.400	1.400 peak 25012 weight	0.10000E+01 volume	0.42103E+03 ppm1	2.466 ppm2	7.519	3.916 ppm2	2.206
((segid "BRD" and resid 21 and name H2))									
ASST [25432]	2.400	1.400	1.400 peak 25022 weight	0.10000E+01 volume	0.12193E+03 ppm1	1.448 ppm2	7.511	3.670 ppm2	7.893
((segid "BRD" and resid 21 and name H2))									
ASST [25432]	2.400	1.400	1.400 peak 25032 weight	0.10000E+01 volume	0.15768E+03 ppm1	1.448 ppm2	1.746	3.917 ppm2	7.778
((segid "BRD" and resid 21 and name H2))									
ASST [25432]	2.200	1.200	1.200 peak 25082 weight	0.10000E+01 volume	0.65457E+03 ppm1	2.316 ppm2	1.746	1.551 ppm2	4.532
((segid "BRD" and resid 17 and name H2))									
ASST [25432]	3.400	1.700	1.700 peak 25092 weight	0.10000E+01 volume	0.25380E+02 ppm1	2.336 ppm2	1.322	1.549 ppm2	4.932
((segid "BRD" and resid 102 and name H2))									
OR [25432]									
ASST [25432]	3.300	2.700	2.200 peak 25102 weight	0.10000E+01 volume	0.61177E+03 ppm1	1.448 ppm2	4.647	1.599 ppm2	0.408
((segid "BRD" and resid 21 and name H2))									
ASST [25432]	2.200	1.200	1.200 peak 25112 weight	0.10000E+01 volume	0.61198E+03 ppm1	2.336 ppm2	1.498	1.599 ppm2	3.069
((segid "BRD" and resid 21 and name H2))									
ASST [25432]	2.200	2.000	2.000 peak 25122 weight	0.10000E+01 volume	0.17749E+03 ppm1	1.205 ppm2	1.312	1.599 ppm2	3.012
((segid "BRD" and resid 21 and name H2))									
ASST [25432]	3.400	2.900	2.900 peak 25102 weight	0.10000E+01 volume	0.54202E+02 ppm1	1.205 ppm2	0.902	1.599 ppm2	2.157
((segid "BRD" and resid 21 and name H2))									
ASST [25432]	2.400	2.000	2.000 peak 25122 weight	0.10000E+01 volume	0.17480E+03 ppm1	1.599 ppm2	7.638	1.549 ppm2	1.970
((segid "BRD" and resid 21 and name H2))									
ASST [25432]	3.500	3.100	2.000 peak 25102 weight	0.10000E+01 volume	0.42795E+02 ppm1	1.599 ppm2	6.998	2.336 ppm2	1.410
((segid "BRD" and resid 101 and name H2))									
ASST [25432]	3.500	3.100	2.000 peak 25112 weight	0.10000E+01 volume	0.43188E+02 ppm1	1.599 ppm2	5.444	1.497 ppm2	0.676
((segid "BRD" and resid 101 and name H2))									
ASST [25432]	2.900	2.900	2.100 peak 25122 weight	0.10000E+01 volume	0.52950E+02 ppm1	4.261 ppm2	4.948	1.155 ppm2	7.529
((segid "BRD" and resid 101 and name H2))									
ASST [25432]	3.100	2.400	2.400 peak 25132 weight	0.10000E+01 volume	0.87416E+02 ppm1	4.261 ppm2	3.475	1.155 ppm2	2.182
((segid "BRD" and resid 101 and name H2))									
ASST [25432]	3.300	3.100	2.000 peak 25162 weight	0.10000E+01 volume	0.47110E+02 ppm1	2.536 ppm2	4.525	1.351 ppm2	7.789
((segid "BRD" and resid 98 and name H2))									
ASST [25432]	5.100	5.100	0.400 peak 25382 weight	0.10000E+01 volume	0.45668E+01 ppm1	4.404 ppm2	1.311	1.155 ppm2	7.529
((segid "BRD" and resid 102 and name H2))									
ASST [25402]									
((segid "BRD" and resid 98 and name H2))									

—

60

—

ASST (3224)
 ((segid "BPD" and read 42 and name H01))
 ((segid "BPD" and read 43 and name H01))
 ((segid "BPD" and read 44 and name H01))
 2.900 2.100 2.100 peak 4204 weight 0.10000E+01 volume 0.2235E+03 ppm1 7.714 ppm2 1.544

ASST (3225)
 ((segid "BPD" and read 45 and name H01))
 ((segid "BPD" and read 46 and name H01))
 ((segid "BPD" and read 47 and name H01))
 2.500 1.600 1.600 peak 4264 weight 0.10000E+01 volume 0.4855E+03 ppm1 7.781 ppm2 4.993

ASST (3226)
 ((segid "BPD" and read 48 and name H01))
 ((segid "BPD" and read 49 and name H01))
 ((segid "BPD" and read 50 and name H01))
 2.500 1.600 1.600 peak 4304 weight 0.10000E+01 volume 0.2778E+03 ppm1 7.802 ppm2 7.517

ASST (3227)
 ((segid "BPD" and read 51 and name H01))
 ((segid "BPD" and read 52 and name H01))
 ((segid "BPD" and read 53 and name H01))
 3.300 2.700 2.700 peak 4324 weight 0.10000E+01 volume 0.9457E+02 ppm1 7.031 ppm2 3.790

ASST (3228)
 ((segid "BPD" and read 54 and name H01))
 ((segid "BPD" and read 55 and name H01))
 ((segid "BPD" and read 56 and name H01))
 3.400 2.900 2.900 peak 4364 weight 0.10000E+01 volume 0.7823E+02 ppm1 7.888 ppm2 1.085

ASST (3229)
 ((segid "BPD" and read 57 and name H01))
 ((segid "BPD" and read 58 and name H01))
 ((segid "BPD" and read 59 and name H01))
 2.800 1.700 1.700 peak 4404 weight 0.11000E+01 volume 0.1452E+03 ppm1 4.028 ppm2 1.081

ASST (3230)
 ((segid "BPD" and read 60 and name H01))
 ((segid "BPD" and read 61 and name H01))
 ((segid "BPD" and read 62 and name H01))
 2.800 1.700 1.700 peak 4444 weight 0.11000E+01 volume 0.1452E+03 ppm1 4.028 ppm2 0.723

ASST (3231)
 ((segid "BPD" and read 63 and name H01))
 ((segid "BPD" and read 64 and name H01))
 ((segid "BPD" and read 65 and name H01))
 2.800 1.700 1.700 peak 4484 weight 0.11000E+01 volume 0.1452E+03 ppm1 4.028 ppm2 1.409

ASST (3232)
 ((segid "BPD" and read 66 and name H01))
 ((segid "BPD" and read 67 and name H01))
 ((segid "BPD" and read 68 and name H01))
 2.800 1.700 1.700 peak 4524 weight 0.11000E+01 volume 0.1452E+03 ppm1 4.028 ppm2 1.401

ASST (3233)
 ((segid "BPD" and read 69 and name H01))
 ((segid "BPD" and read 70 and name H01))
 ((segid "BPD" and read 71 and name H01))
 2.800 1.700 1.700 peak 4564 weight 0.11000E+01 volume 0.1452E+03 ppm1 4.028 ppm2 1.074

ASST (3234)
 ((segid "BPD" and read 72 and name H01))
 ((segid "BPD" and read 73 and name H01))
 ((segid "BPD" and read 74 and name H01))
 2.800 1.700 1.700 peak 4604 weight 0.11000E+01 volume 0.1452E+03 ppm1 4.028 ppm2 1.408

ASST (3235)
 ((segid "BPD" and read 75 and name H01))
 ((segid "BPD" and read 76 and name H01))
 ((segid "BPD" and read 77 and name H01))
 2.800 1.700 1.700 peak 4644 weight 0.11000E+01 volume 0.1452E+03 ppm1 4.028 ppm2 1.592

ASST (3236)
 ((segid "BPD" and read 78 and name H01))
 ((segid "BPD" and read 79 and name H01))
 ((segid "BPD" and read 80 and name H01))
 2.800 1.700 1.700 peak 4684 weight 0.11000E+01 volume 0.1452E+03 ppm1 4.028 ppm2 1.066

ASST (3237)
 ((segid "BPD" and read 81 and name H01))
 ((segid "BPD" and read 82 and name H01))
 ((segid "BPD" and read 83 and name H01))
 2.800 1.700 1.700 peak 4724 weight 0.11000E+01 volume 0.1452E+03 ppm1 4.028 ppm2 0.491

ASST (3238)
 ((segid "BPD" and read 84 and name H01))
 ((segid "BPD" and read 85 and name H01))
 ((segid "BPD" and read 86 and name H01))
 2.800 1.700 1.700 peak 4764 weight 0.11000E+01 volume 0.1452E+03 ppm1 4.028 ppm2 0.727

ASST (3239)
 ((segid "BPD" and read 87 and name H01))
 ((segid "BPD" and read 88 and name H01))
 ((segid "BPD" and read 89 and name H01))
 2.800 1.700 1.700 peak 4804 weight 0.11000E+01 volume 0.1452E+03 ppm1 4.028 ppm2 1.072

ASST (3240)
 ((segid "BPD" and read 90 and name H01))
 ((segid "BPD" and read 91 and name H01))
 ((segid "BPD" and read 92 and name H01))
 2.800 1.700 1.700 peak 4844 weight 0.11000E+01 volume 0.1452E+03 ppm1 4.028 ppm2 1.403

ASST (3241)
 ((segid "BPD" and read 93 and name H01))
 ((segid "BPD" and read 94 and name H01))
 ((segid "BPD" and read 95 and name H01))
 2.800 1.700 1.700 peak 4884 weight 0.11000E+01 volume 0.1452E+03 ppm1 4.028 ppm2 4.209

ASST (3242)
 ((segid "BPD" and read 96 and name H01))
 ((segid "BPD" and read 97 and name H01))
 ((segid "BPD" and read 98 and name H01))
 2.800 1.700 1.700 peak 4924 weight 0.11000E+01 volume 0.1452E+03 ppm1 4.028 ppm2 5.520

ASST (3243)
 ((segid "BPD" and read 99 and name H01))
 ((segid "BPD" and read 100 and name H01))
 ((segid "BPD" and read 101 and name H01))
 2.800 1.700 1.700 peak 4964 weight 0.11000E+01 volume 0.1452E+03 ppm1 4.028 ppm2 4.448

```

(( segid "ACH" - and resid 201 and name HA2 ))
ASSI ( 34 )
(( segid "BPD" - and resid 86 and name HA1 ))
(( segid "ACH" - and resid 201 and name HA2 ))
(( segid "BPD" - and resid 95 and name HA1 ))
OR ( 3700 1.800 1.800 peak 16 weight 0.110008*01 volume 0.119248*03 ppm1 4.015 ppm2 7.461
(( segid "ACH" - and resid 201 and name HA1 ))
(( segid "BPD" - and resid 95 and name HA1 ))
ASSI ( 24 )
(( segid "ACH" - and resid 201 and name HA1 ))
(( segid "BPD" - and resid 95 and name HA1 ))
OR ( 2400 1.700 1.700 peak 36 weight 0.110008*01 volume 0.152298*03 ppm1 3.439 ppm2 7.461
(( segid "ACH" - and resid 201 and name HA2 ))
(( segid "BPD" - and resid 95 and name HA1 ))
ASSI ( 36 )
(( segid "ACH" - and resid 201 and name HA1 ))
(( segid "BPD" - and resid 88 and name HA1 ))
OR ( 2400 1.800 1.800 peak 36 weight 0.110008*01 volume 0.184658*03 ppm1 4.015 ppm2 7.637
(( segid "ACH" - and resid 201 and name HA2 ))
(( segid "BPD" - and resid 88 and name HA1 ))
ASSI ( 46 )
(( segid "ACH" - and resid 201 and name HA2 ))
(( segid "BPD" - and resid 88 and name HA1 ))
OR ( 2400 1.800 1.800 peak 46 weight 0.110008*01 volume 0.139386*03 ppm1 3.439 ppm2 7.637
(( segid "ACH" - and resid 201 and name HA1 ))
(( segid "BPD" - and resid 88 and name HA1 ))
ASSI ( 56 )
(( segid "ACH" - and resid 201 and name HA2 ))
(( segid "BPD" - and resid 88 and name HA1 ))
OR ( 2400 1.700 1.700 peak 56 weight 0.110008*01 volume 0.160758*03 ppm1 4.015 ppm2 7.585
(( segid "ACH" - and resid 201 and name HA1 ))
(( segid "BPD" - and resid 95 and name HA1 ))
ASSI ( 66 )
(( segid "ACH" - and resid 201 and name HA1 ))
(( segid "BPD" - and resid 85 and name HA1 ))
OR ( 2400 1.700 1.700 peak 66 weight 0.110008*01 volume 0.149738*03 ppm1 3.439 ppm2 7.585
(( segid "ACH" - and resid 200 and name HA1 ))
(( segid "BPD" - and resid 95 and name HA1 ))
ASSI ( 86 )
(( segid "ACH" - and resid 201 and name HA1 ))
(( segid "BPD" - and resid 86 and name HA1 ))
OR ( 2400 1.700 1.700 peak 86 weight 0.110008*01 volume 0.140498*03 ppm1 2.542 ppm2 7.585
(( segid "ACH" - and resid 201 and name HA1 ))
(( segid "BPD" - and resid 86 and name HA1 ))
OR ( 2400 1.700 1.700 peak 86 weight 0.110008*01 volume 0.167968*03 ppm1 4.019 ppm2 7.358
(( segid "ACH" - and resid 201 and name HA2 ))
(( segid "BPD" - and resid 88 and name HA1 ))
ASSI ( 96 )
(( segid "ACH" - and resid 201 and name HA2 ))
(( segid "BPD" - and resid 88 and name HA1 ))
OR ( 2400 1.700 1.700 peak 96 weight 0.110008*01 volume 0.157638*03 ppm1 3.430 ppm2 7.358
(( segid "ACH" - and resid 200 and name HA1 ))
(( segid "BPD" - and resid 201 and name HA1 ))
ASSI ( 7 )
(( segid "ACH" - and resid 200 and name HA1 ))
(( segid "ACH" - and resid 201 and name HA1 ))
(( segid "BPD" - and resid 201 and name HA1 ))
OR ( 2400 1.800 1.800 peak 7 weight 0.110008*01 volume 0.120008*03 ppm1 3.430 ppm2 7.358
(( segid "ACH" - and resid 200 and name HA1 ))
(( segid "BPD" - and resid 201 and name HA1 ))
ASSI ( 27 )
(( segid "ACH" - and resid 201 and name HA2 ))
(( segid "ACH" - and resid 201 and name HA1 ))
(( segid "BPD" - and resid 201 and name HA1 ))
OR ( 2400 1.800 1.800 peak 27 weight 0.110008*01 volume 0.120008*03 ppm1 3.430 ppm2 7.358
(( segid "ACH" - and resid 201 and name HA1 ))
(( segid "BPD" - and resid 201 and name HA1 ))
ASSI ( 37 )
(( segid "ACH" - and resid 201 and name HA1 ))
(( segid "ACH" - and resid 201 and name HA1 ))
(( segid "BPD" - and resid 201 and name HA1 ))
OR ( 2400 1.800 1.800 peak 37 weight 0.110008*01 volume 0.120008*03 ppm1 3.430 ppm2 7.358
(( segid "ACH" - and resid 201 and name HA2 ))
(( segid "BPD" - and resid 201 and name HA1 ))
ASSI ( 47 )
(( segid "ACH" - and resid 201 and name HA2 ))
(( segid "ACH" - and resid 201 and name HA1 ))
(( segid "BPD" - and resid 201 and name HA1 ))
OR ( 2400 1.800 1.800 peak 47 weight 0.110008*01 volume 0.120008*03 ppm1 3.430 ppm2 7.358
(( segid "ACH" - and resid 201 and name HA1 ))
(( segid "BPD" - and resid 201 and name HA1 ))

```


2

OR { 79611 ((segid "BFD" * and resaid 18 and name HB1)) ((segid "BFD" * and resaid 103 and name HN)) ((segid "BFD" * and resaid 104 and name HO1)) ASSI { 10091 ((segid "BFD" * and resaid 24 and name HN)) ((segid "BFD" * and resaid 21 and name HB)) ((segid "BFD" * and resaid 11 and name HO1)) 4 300 4 300 1 200 peak 10081 weight 0 100008*01 volume 0 28058*02 ppm1		2 481	8 666 ppm2
OR { 10081 ((segid "BFD" * and resaid 24 and name HN)) ((segid "BFD" * and resaid 26 and name HB1)) ASSI { 10181 ((segid "BFD" * and resaid 16 and name HN)) ((segid "BFD" * and resaid 14 and name HB2)) ((segid "BFD" * and resaid 14 and name HB2)) 4 100 4 100 1 400 peak 10181 weight 0 100008*01 volume 0 40566*02 ppm1		2 129	0 785 ppm2
OR { 10191 ((segid "BFD" * and resaid 16 and name HN)) ((segid "BFD" * and resaid 18 and name HB1)) ASSI { 10201 ((segid "BFD" * and resaid 16 and name HN)) ((segid "BFD" * and resaid 13 and name HB2)) ((segid "BFD" * and resaid 13 and name HB2)) 3 800 1 600 peak 10201 weight 0 100008*01 volume 0 579318*02 ppm1		1 963	8 791 ppm2
OR { 10201 ((segid "BFD" * and resaid 16 and name HN)) ((segid "BFD" * and resaid 13 and name HB2)) ASSI { 10241 ((segid "BFD" * and resaid 75 and name HN)) ((segid "BFD" * and resaid 75 and name HB1)) ((segid "BFD" * and resaid 75 and name HB1)) 3 900 1 800 1 600 peak 10241 weight 0 100008*01 volume 0 500508*02 ppm1		1 347	9 106 ppm2
OR { 10281 ((segid "BFD" * and resaid 75 and name HN)) ((segid "BFD" * and resaid 115 and name HO1A)) ASSI { 10291 ((segid "BFD" * and resaid 98 and name HN)) ((segid "BFD" * and resaid 97 and name HO1)) 4 000 4 000 1 500 peak 10291 weight 0 100008*01 volume 0 433238*02 ppm1		2 456	9 106 ppm2
OR { 10301 ((segid "BFD" * and resaid 98 and name HN)) ((segid "BFD" * and resaid 97 and name HO1)) OR { 10311 ((segid "BFD" * and resaid 98 and name HN)) ((segid "BFD" * and resaid 101 and name HO1)) ASSI { 10331 ((segid "BFD" * and resaid 96 and name HN)) ((segid "BFD" * and resaid 96 and name HB1)) ((segid "BFD" * and resaid 96 and name HB1)) 3 800 1 600 peak 10331 weight 0 100008*01 volume 0 522458*02 ppm1		2 412	7 977 ppm2
OR { 10331 ((segid "BFD" * and resaid 77 and name HN)) ((segid "BFD" * and resaid 71 and name HO)) OR { 10341 ((segid "BFD" * and resaid 96 and name HN)) ((segid "BFD" * and resaid 97 and name HO1)) OR { 10351 ((segid "BFD" * and resaid 77 and name HN)) ((segid "BFD" * and resaid 72 and name HB1)) ASSI { 10391 ((segid "BFD" * and resaid 78 and name HN)) ((segid "BFD" * and resaid 116 and name HO1)) ((segid "BFD" * and resaid 116 and name HO1)) 3 900 3 800 1 600 peak 10391 weight 0 100008*01 volume 0 515458*02 ppm1		1 888	7 996 ppm2
OR { 10391 ((segid "BFD" * and resaid 77 and name HN)) ((segid "BFD" * and resaid 116 and name HO1)) ASSI { 10401 ((segid "BFD" * and resaid 78 and name HN)) ((segid "BFD" * and resaid 78 and name HO2A)) ((segid "BFD" * and resaid 22 and name HO2A)) 3 500 3 100 2 000 peak 10391 weight 0 100008*01 volume 0 932098*02 ppm1		1 604	7 996 ppm2
OR { 10391 ((segid "BFD" * and resaid 55 and name HN)) ((segid "BFD" * and resaid 22 and name HO2A)) OR { 10401 ((segid "BFD" * and resaid 55 and name HN)) ((segid "BFD" * and resaid 22 and name HO2A)) ASSI { 10411 ((segid "BFD" * and resaid 77 and name HN)) ((segid "BFD" * and resaid 77 and name HB2)) ((segid "BFD" * and resaid 77 and name HB2)) 2 000 2 000 2 000 peak 10411 weight 0 100008*01 volume 0 431958*02 ppm1		2 456	7 996 ppm2
OR { 10411 ((segid "BFD" * and resaid 78 and name HN)) ((segid "BFD" * and resaid 80 and name HB2)) ASSI { 10431 ((segid "BFD" * and resaid 55 and name HN)) ((segid "BFD" * and resaid 77 and name HO1)) ((segid "BFD" * and resaid 77 and name HO1)) 2 600 1 700 1 700 peak 10431 weight 0 100008*01 volume 0 603648*02 ppm1		2 722	7 996 ppm2

5

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	120	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	144	145	146	147	148	149	150	151	152	153	154	155	156	157	158	159	160	161	162	163	164	165	166	167	168	169	170	171	172	173	174	175	176	177	178	179	180	181	182	183	184	185	186	187	188	189	190	191	192	193	194	195	196	197	198	199	200	201	202	203	204	205	206	207	208	209	210	211	212	213	214	215	216	217	218	219	220	221	222	223	224	225	226	227	228	229	230	231	232	233	234	235	236	237	238	239	240	241	242	243	244	245	246	247	248	249	250	251	252	253	254	255	256	257	258	259	260	261	262	263	264	265	266	267	268	269	270	271	272	273	274	275	276	277	278	279	280	281	282	283	284	285	286	287	288	289	290	291	292	293	294	295	296	297	298	299	300	301	302	303	304	305	306	307	308	309	310	311	312	313	314	315	316	317	318	319	320	321	322	323	324	325	326	327	328	329	330	331	332	333	334	335	336	337	338	339	340	341	342	343	344	345	346	347	348	349	350	351	352	353	354	355	356	357	358	359	360	361	362	363	364	365	366	367	368	369	370	371	372	373	374	375	376	377	378	379	380	381	382	383	384	385	386	387	388	389	390	391	392	393	394	395	396	397	398	399	400	401	402	403	404	405	406	407	408	409	410	411	412	413	414	415	416	417	418	419	420	421	422	423	424	425	426	427	428	429	430	431	432	433	434	435	436	437	438	439	440	441	442	443	444	445	446	447	448	449	450	451	452	453	454	455	456	457	458	459	460	461	462	463	464	465	466	467	468	469	470	471	472	473	474	475	476	477	478	479	480	481	482	483	484	485	486	487	488	489	490	491	492	493	494	495	496	497	498	499	500	501	502	503	504	505	506	507	508	509	510	511	512	513	514	515	516	517	518	519	520	521	522	523	524	525
---	---	---	---	---	---	---	---	---	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

2

Year	1990	1991	1992	1993	1994	1995	1996	1997	1998	1999	2000	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018	2019	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030	2031	2032	2033	2034	2035	2036	2037	2038	2039	2040	2041	2042	2043	2044	2045	2046	2047	2048	2049	2050	2051	2052	2053	2054	2055	2056	2057	2058	2059	2060	2061	2062	2063	2064	2065	2066	2067	2068	2069	2070	2071	2072	2073	2074	2075	2076	2077	2078	2079	2080	2081	2082	2083	2084	2085	2086	2087	2088	2089	2090	2091	2092	2093	2094	2095	2096	2097	2098	2099	2100
1990	1991	1992	1993	1994	1995	1996	1997	1998	1999	2000	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018	2019	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030	2031	2032	2033	2034	2035	2036	2037	2038	2039	2040	2041	2042	2043	2044	2045	2046	2047	2048	2049	2050	2051	2052	2053	2054	2055	2056	2057	2058	2059	2060	2061	2062	2063	2064	2065	2066	2067	2068	2069	2070	2071	2072	2073	2074	2075	2076	2077	2078	2079	2080	2081	2082	2083	2084	2085	2086	2087	2088	2089	2090	2091	2092	2093	2094	2095	2096	2097	2098	2099	2100	

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	120	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	144	145	146	147	148	149	150	151	152	153	154	155	156	157	158	159	160	161	162	163	164	165	166	167	168	169	170	171	172	173	174	175	176	177	178	179	180	181	182	183	184	185	186	187	188	189	190	191	192	193	194	195	196	197	198	199	200	201	202	203	204	205	206	207	208	209	210	211	212	213	214	215	216	217	218	219	220	221	222	223	224	225	226	227	228	229	230	231	232	233	234	235	236	237	238	239	240	241	242	243	244	245	246	247	248	249	250	251	252	253	254	255	256	257	258	259	260	261	262	263	264	265	266	267	268	269	270	271	272	273	274	275	276	277	278	279	280	281	282	283	284	285	286	287	288	289	290	291	292	293	294	295	296	297	298	299	300	301	302	303	304	305	306	307	308	309	310	311	312	313	314	315	316	317	318	319	320	321	322	323	324	325	326	327	328	329	330	331	332	333	334	335	336	337	338	339	340	341	342	343	344	345	346	347	348	349	350	351	352	353	354	355	356	357	358	359	360	361	362	363	364	365	366	367	368	369	370	371	372	373	374	375	376	377	378	379	380	381	382	383	384	385	386	387	388	389	390	391	392	393	394	395	396	397	398	399	400	401	402	403	404	405	406	407	408	409	410	411	412	413	414	415	416	417	418	419	420	421	422	423	424	425	426	427	428	429	430	431	432	433	434	435	436	437	438	439	440	441	442	443	444	445	446	447	448	449	450	451	452	453	454	455	456	457	458	459	460	461	462	463	464	465	466	467	468	469	470	471	472	473	474	475	476	477	478	479	480	481	482	483	484	485	486	487	488	489	490	491	492	493	494	495	496	497	498	499	500	501	502	503	504	505	506	507	508	509	510	511	512	513	514	515	516	517	518	519	520	521	522	523	524	525
---	---	---	---	---	---	---	---	---	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

Figure 1 consists of 12 histograms arranged in a single column. Each histogram represents the distribution of the number of non-zero elements in the vector x for a specific value of n . The x-axis for all histograms is labeled 'x' and ranges from 0 to 120. The y-axis is labeled 'count' and ranges from 0 to 1000. The histograms are for $n = 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 110, 120$. As n increases, the distribution of non-zero elements shifts to the right, indicating that more elements in the vector x are non-zero for larger n . The peak count for each distribution decreases as n increases.

```
(( segid = end read 56 and name HQ1 ))  
(( segid "BrD" = and read 81  
and name HG2 ))  
OK {7862}  
{{ segid "BrD" = and read 76  
and name HB2 }}
```


0	10000E+01	volume	0	43603E+03	pptm1
0	10000E+01	volume	0	15243E+04	pptm1
0	10000E+01	volume	0	54441E+03	pptm1
0	10000E+01	volume	0	50159E+02	pptm1
0	10000E+01	volume	0	12304E+03	pptm1
0	10000E+01	volume	0	47618E+03	pptm1
0	10000E+01	volume	0	54491E+03	pptm1
0	10000E+01	volume	0	30683E+03	pptm1
0	10000E+01	volume	0	84175E+03	pptm1
0	10000E+01	volume	0	45504E+03	pptm1

Variable	Mean	SD	Min	Max
Age	42.2	10.5	22	65
Gender	65.6	47.8	0	100
Marital status	60.0	49.2	0	100
Education	93.6	22.4	70	100
Income	57.0	25.3	30	80
Health status	67.4	27.1	40	90
Religious belief	81.9	28.5	60	100
Life satisfaction	57.8	27.8	30	80
Depression	-0.10	0.79	-1	1
Loneliness	.796	0.40	0	1

[illegible]

26

[illegible]

Variable	Mean	Standard deviation	Minimum	Maximum
Age	35.5	10.5	20	55
Gender	0.5	0.5	0	1
Marital status	0.5	0.5	0	1
Education	12.5	1.5	10	15
Income	15.5	5.5	10	25
Health status	0.5	0.5	0	1
Smoking status	0.5	0.5	0	1
Alcohol consumption	0.5	0.5	0	1
Exercise frequency	0.5	0.5	0	1
Stress level	0.5	0.5	0	1
Sleep quality	0.5	0.5	0	1
Work satisfaction	0.5	0.5	0	1
Life satisfaction	0.5	0.5	0	1
Overall health	0.5	0.5	0	1

Table 4

Hydrogen Bonding Restraints

```

!Helix Z
assign (residue 19 and name HN ) (residue 15 and name O ) 1.80 0.0 0.40
assign (residue 19 and name N ) (residue 15 and name O ) 2.80 0.30 0.40

assign (residue 22 and name HN ) (residue 18 and name O ) 1.80 0.0 0.40
assign (residue 22 and name N ) (residue 18 and name O ) 2.80 0.30 0.40

assign (residue 23 and name HN ) (residue 19 and name O ) 1.80 0.0 0.40
assign (residue 23 and name N ) (residue 19 and name O ) 2.80 0.30 0.40

assign (residue 24 and name HN ) (residue 20 and name O ) 1.80 0.0 0.40
assign (residue 24 and name N ) (residue 20 and name O ) 2.80 0.30 0.40

assign (residue 25 and name HN ) (residue 21 and name O ) 1.80 0.0 0.40
assign (residue 25 and name N ) (residue 21 and name O ) 2.80 0.30 0.40

!Helix B
assign (residue 75 and name HN ) (residue 71 and name O ) 1.80 0.0 0.40
assign (residue 75 and name N ) (residue 71 and name O ) 2.80 0.30 0.40

!assign (residue 77 and name HN ) (residue 73 and name O ) 1.80 0.0 0.40
!assign (residue 77 and name N ) (residue 73 and name O ) 2.80 0.30 0.40

assign (residue 78 and name HN ) (residue 74 and name O ) 1.80 0.0 0.40
assign (residue 78 and name N ) (residue 74 and name O ) 2.80 0.30 0.40

assign (residue 79 and name HN ) (residue 75 and name O ) 1.80 0.0 0.40
assign (residue 79 and name N ) (residue 75 and name O ) 2.80 0.30 0.40

!assign (residue 80 and name HN ) (residue 76 and name O ) 1.80 0.0 0.40
!assign (residue 80 and name N ) (residue 76 and name O ) 2.80 0.30 0.40

assign (residue 81 and name HN ) (residue 77 and name O ) 1.80 0.0 0.40
assign (residue 81 and name N ) (residue 77 and name O ) 2.80 0.30 0.40

assign (residue 82 and name HN ) (residue 78 and name O ) 1.80 0.0 0.40
assign (residue 82 and name N ) (residue 78 and name O ) 2.80 0.30 0.40

!Helix C
assign (residue 102 and name HN ) (residue 98 and name O ) 1.80 0.0 0.40
assign (residue 102 and name N ) (residue 98 and name O ) 2.80 0.30 0.40

assign (residue 103 and name HN ) (residue 99 and name O ) 1.80 0.0 0.40
assign (residue 103 and name N ) (residue 99 and name O ) 2.80 0.30 0.40

assign (residue 104 and name HN ) (residue 100 and name O ) 1.80 0.0 0.40
assign (residue 104 and name N ) (residue 100 and name O ) 2.80 0.30 0.40

assign (residue 105 and name HN ) (residue 101 and name O ) 1.80 0.0 0.40
assign (residue 105 and name N ) (residue 101 and name O ) 2.80 0.30 0.40

```

Atomic Structure Coordinates of the Free Form of the P/CAF Bromodomain

1

[illegible]

3

[illegible]

5

ATOM	1363	CDI	TWR	83	-4.464	7.246	-6.519	1.00	0.00	ATOM	1571	O	TWR	95	-10.170	6.352	2.951	1.00	0.00
ATOM	1364	H02	THR	83	-3.454	7.404	-6.329	1.00	0.00	ATOM	1572	NN	TWR	96	-11.743	7.934	1.243	1.00	0.00
ATOM	1365	H02	THR	83	-8.255	-6.349	1.00	0.00	0.00	ATOM	1573	NN	TWR	96	-12.486	8.045	1.432	1.00	0.00
ATOM	1366	H02	THR	83	-5.228	6.255	-6.049	1.00	0.00	ATOM	1574	CA	TWR	96	-10.816	8.265	3.073	1.00	0.00
ATOM	1367	C	THR	83	-6.278	-6.017	-3.711	1.00	0.00	ATOM	1575	CA	TWR	96	-10.140	7.248	2.288	1.00	0.00
ATOM	1368	O	THR	83	-7.231	6.740	-6.013	1.00	0.00	ATOM	1576	HH	TWR	96	-12.376	10.073	2.027	1.00	0.00
ATOM	1369	NN	ASN	84	-5.550	4.370	-3.476	1.00	0.00	ATOM	1577	HH	TWR	96	-12.376	10.073	2.027	1.00	0.00
ATOM	1370	NN	ASN	84	-7.523	3.987	-4.150	1.00	0.00	ATOM	1578	H02	TWR	96	-10.101	10.145	3.611	1.00	0.00
ATOM	1391	CA	ASN	84	-7.320	4.381	-5.153	1.00	0.00	ATOM	1579	CA	TWR	96	-10.717	11.378	2.060	1.00	0.00
ATOM	1392	HA	ASN	84	-7.250	2.431	-4.321	1.00	0.00	ATOM	1580	CA	TWR	96	-10.257	11.219	0.759	1.00	0.00
ATOM	1393	CA	ASN	84	-6.457	2.142	-5.019	1.00	0.00	ATOM	1581	HH	ASN	96	-10.344	10.745	3.745	1.00	0.00
ATOM	1394	HH	ASN	84	-6.457	2.142	-5.019	1.00	0.00	ATOM	1582	CDI	TWR	96	-10.344	10.745	3.745	1.00	0.00
ATOM	1395	HH	ASN	84	-6.457	2.142	-5.019	1.00	0.00	ATOM	1583	H02	TWR	96	-10.714	12.672	3.758	1.00	0.00
ATOM	1396	C	ASN	84	-8.468	4.707	-4.718	1.00	0.00	ATOM	1584	CDI	TWR	96	-9.471	12.183	0.159	1.00	0.00
ATOM	1397	H02	ASN	84	-9.459	2.282	-5.218	1.00	0.00	ATOM	1585	HH	TWR	96	-9.120	12.039	-0.952	1.00	0.00
ATOM	1398	H02	ASN	84	-8.368	0.385	-4.672	1.00	0.00	ATOM	1586	CDI	TWR	96	-9.576	12.501	2.522	1.00	0.00
ATOM	1399	H02	ASN	84	-7.564	-0.004	-4.312	1.00	0.00	ATOM	1587	HH	TWR	96	-9.111	11.320	0.701	1.00	0.00
ATOM	1400	H02	ASN	84	-9.156	-0.147	-4.960	1.00	0.00	ATOM	1588	CA	TWR	96	-9.111	11.320	0.701	1.00	0.00
ATOM	1401	CA	ASN	84	-9.156	-0.147	-4.960	1.00	0.00	ATOM	1589	CA	TWR	96	-8.347	14.282	0.365	1.00	0.00
ATOM	1402	C	ASN	84	-9.656	4.879	-3.514	1.00	0.00	ATOM	1590	HH	TWR	96	-6.832	14.690	-0.456	1.00	0.00
ATOM	1403	N	CYS	85	-8.520	3.657	-2.003	1.00	0.00	ATOM	1591	C	TWR	96	-10.009	9.267	4.346	1.00	0.00
ATOM	1404	HN	CYS	85	-7.708	3.182	-1.812	1.00	0.00	ATOM	1592	O	TWR	96	-8.884	9.764	4.303	1.00	0.00
ATOM	1405	CA	CYS	85	-9.526	3.808	-0.941	1.00	0.00	ATOM	1593	CA	LVS	97	-9.515	10.043	6.906	1.00	0.00
ATOM	1406	HN	CYS	85	-10.024	3.285	-0.356	1.00	0.00	ATOM	1594	NN	LVS	97	-10.457	9.033	4.545	1.00	0.00
ATOM	1407	HN	CYS																

ATOM	1665	H012	ILE	101	-6.475	5.842	11.709	1.00	0.00	1.491	2.500	3.935	2.853	0.471	1.00	0.00	7.830	11.569	3.543	1.50	0.00	ATOM	1653	NZ	LVS	111	7.340	11.167	1.560	1.00	0.00
ATOM	1666	H013	ILE	101	-7.094	5.966	10.534	1.00	0.00	1.935	2.853	3.935	2.853	0.471	1.00	0.00	7.340	11.569	3.543	1.50	0.00	ATOM	1654	NZ	LVS	111	7.340	11.569	3.543	1.50	0.00
ATOM	1667	C	ILE	101	-2.311	6.457	8.226	1.00	0.00	4.605	3.334	1.814	1.00	0.00	1.00	0.00	7.131	10.573	2.187	1.00	0.00	ATOM	1655	H02	LVS	111	7.131	10.573	2.187	1.00	0.00
ATOM	1668	C	ILE	101	-1.335	6.507	8.232	1.00	0.00	5.125	0.780	1.050	1.00	0.00	1.00	0.00	8.121	11.954	2.084	1.00	0.00	ATOM	1656	H02	LVS	111	8.121	11.954	2.084	1.00	0.00
ATOM	1669	C	ILE	101	-2.376	5.343	7.900	1.00	0.00	5.188	5.213	5.110	1.00	0.00	1.00	0.00	12.448	7.070	4.425	1.00	0.00	ATOM	1657	C	LVS	111	12.448	7.070	4.425	1.00	0.00
ATOM	1670	HN	LVS	102	-1.988	4.457	6.972	1.00	0.00	3.795	4.355	4.434	1.00	0.00	1.00	0.00	12.347	6.285	3.487	1.00	0.00	ATOM	1658	HN	LVS	112	12.347	6.285	3.487	1.00	0.00
ATOM	1671	CA	LVS	102	-1.988	4.457	6.972	1.00	0.00	3.795	4.355	4.434	1.00	0.00	1.00	0.00	12.347	6.285	3.487	1.00	0.00	ATOM	1659	CA	LVS	112	12.347	6.285	3.487	1.00	0.00
ATOM	1672	HA	LVS	102	-1.350	3.953	7.763	1.00	0.00	2.814	6.212	4.432	1.00	0.00	1.00	0.00	11.489	6.225	5.963	1.00	0.00	ATOM	1660	HA	LVS	112	11.489	6.225	5.963	1.00	0.00
ATOM	1673	CB	LVS	102	-2.369	3.416	6.082	1.00	0.00	4.575	7.140	4.486	1.00	0.00	1.00	0.00	13.485	5.516	5.963	1.00	0.00	ATOM	1661	CB	LVS	112	13.485	5.516	5.963	1.00	0.00
ATOM	1674	HN	LVS	102	-3.430	3.443	6.283	1.00	0.00	5.076	6.416	2.885	1.00	0.00	1.00	0.00	14.297	6.205	6.161	1.00	0.00	ATOM	1662	HN	LVS	112	14.297	6.205	6.161	1.00	0.00
ATOM	1675	HN	LVS	102	-2.030	3.953	7.763	1.00	0.00	2.814	6.212	4.432	1.00	0.00	1.00	0.00	13.485	5.516	5.963	1.00	0.00	ATOM	1663	HN	LVS	112	13.485	5.516	5.963	1.00	0.00
ATOM	1676	CB	LVS	102	-2.430	3.953	7.763	1.00	0.00	2.814	6.212	4.432	1.00	0.00	1.00	0.00	13.485	5.516	5.963	1.00	0.00	ATOM	1664	CB	LVS	112	13.485	5.516	5.963	1.00	0.00
ATOM	1677	HA	LVS	102	-2.423	1.332	5.420	1.00	0.00	4.263	9.076	2.810	1.00	0.00	1.00	0.00	13.864	4.054	7.509	1.00	0.00	ATOM	1665	HA	LVS	112	13.864	4.054	7.509	1.00	0.00
ATOM	1678	CD	LVS	102	-2.476	1.364	7.523	1.00	0.00	2.918	7.770	1.838	1.00	0.00	1.00	0.00	13.070	5.760	4.889	1.00	0.00	ATOM	1666	CD	LVS	112	13.070	5.760	4.889	1.00	0.00
ATOM	1679	H011	LVS	102	-1.943	1.335	8.316	1.00	0.																						

ATOM	1947	H82	LVS	118	4.432	9.001	-5.028	1.00	0.00
ATOM	1948	CS	LVS	118	3.021	10.506	-5.527	1.00	0.00
ATOM	1949	H81	LVS	118	3.775	10.146	-6.321	1.00	0.00
ATOM	1950	H83	LVS	118	3.075	10.146	-6.321	1.00	0.00
ATOM	1951	CD	LVS	118	1.642	10.081	-5.053	1.00	0.00
ATOM	1952	H81	LVS	118	1.432	9.100	-5.449	1.00	0.00
ATOM	1953	H82	LVS	118	1.437	10.044	-3.974	1.00	0.00
ATOM	1954	CS	LVS	118	0.569	11.052	-5.518	1.00	0.00
ATOM	1955	H81	LVS	118	-0.025	11.347	-4.688	1.00	0.00
ATOM	1956	H82	LVS	118	-0.025	11.347	-4.688	1.00	0.00
ATOM	1957	H2	LVS	118	-0.324	10.443	-4.843	1.00	0.00
ATOM	1958	H21	LVS	118	-0.734	9.558	-4.180	1.00	0.00
ATOM	1959	H22	LVS	118	0.214	10.214	-7.408	1.00	0.00
ATOM	1960	H23	LVS	118	-1.097	11.099	-6.778	1.00	0.00
ATOM	1961	C	LVS	118	4.976	12.103	-3.687	1.00	0.00
ATOM	1962	OT1	LVS	118	4.967	13.197	-2.291	1.00	0.00
ATOM	1963	OT2	LVS	118	4.901	11.366	-2.463	1.00	0.00
END									

Atomic Structure Coordinates of the P/CAF Bromodomain/Acetyl-Histamine Complex

[illegible]

32	-10.185	-	4.374	-5.123	1.00	0.00	38	-13.457	639 H023 VAL	38	13.365	-4.704	1.00	0.00	721	H02 PRO	44	-17.851
33	-10.859	-	6.429	-6.553	1.00	0.00	39	-10.518	632 C VAL	39	11.298	-4.992	1.00	0.00	722	H03 PRO	45	-18.071
34	-10.646	-	6.431	-6.535	1.00	0.00	40	-10.518	631 C VAL	40	11.298	-4.992	1.00	0.00	723	H04 PRO	46	-18.071
35	-11.693	-	7.488	-8.571	1.00	0.00	41	-11.349	630 C VAL	41	11.337	-4.952	1.00	0.00	724	H05 PRO	47	-17.294
36	-10.747	-	6.433	-6.531	1.00	0.00	42	-10.518	629 C VAL	42	11.337	-4.952	1.00	0.00	725	H06 PRO	48	-17.294
37	-10.747	-	6.433	-6.531	1.00	0.00	43	-10.518	628 C VAL	43	11.337	-4.952	1.00	0.00	726	H07 PRO	49	-17.294
38	-11.926	-	8.737	-8.715	1.00	0.00	44	-11.926	627 C VAL	44	11.337	-4.952	1.00	0.00	727	H08 PRO	50	-17.294
39	-10.771	-	6.433	-6.531	1.00	0.00	45	-10.518	626 C VAL	45	11.337	-4.952	1.00	0.00	728	H09 PRO	51	-17.294
40	-11.713	-	8.737	-8.715	1.00	0.00	46	-11.926	625 C VAL	46	11.337	-4.952	1.00	0.00	729	H10 PRO	52	-17.294
41	-10.771	-	6.433	-6.531	1.00	0.00	47	-10.518	624 C VAL	47	11.337	-4.952	1.00	0.00	730	H11 PRO	53	-17.294
42	-10.771	-	6.433	-6.531	1.00	0.00	48	-10.518	623 C VAL	48	11.337	-4.952	1.00	0.00	731	H12 PRO	54	-17.294
43	-10.771	-	6.433	-6.531	1.00	0.00	49	-10.518	622 C VAL	49	11.337	-4.952	1.00	0.00	732	H13 PRO	55	-17.294
44	-10.771	-	6.433	-6.531	1.00	0.00	50	-10.518	621 C VAL	50	11.337	-4.952	1.00	0.00	733	H14 PRO	56	-17.294
45	-10.771	-	6.433	-6.531	1.00	0.00	51	-10.518	620 C VAL	51	11.337	-4.952	1.00	0.00	734	H15 PRO	57	-17.294
46	-10.771	-	6.433	-6.531	1.00	0.00	52	-10.518	619 C VAL	52	11.337	-4.952	1.00	0.00	735	H16 PRO	58	-17.294
47	-10.771	-	6.433	-6.531	1.00	0.00	53	-10.518	618 C VAL	53	11.337	-4.952	1.00	0.00	736	H17 PRO	59	-17.294
48	-10.771	-	6.433	-6.531	1.00	0.00	54	-10.518	617 C VAL	54	11.337	-4.952	1.00	0.00	737	H18 PRO	60	-17.294
49	-10.771	-	6.433	-6.531	1.00	0.00	55	-10.518	616 C VAL	55	11.337	-4.952	1.00	0.00	738	H19 PRO	61	-17.294
50	-10.771	-	6.433	-6.531	1.00	0.00	56	-10.518	615 C VAL	56	11.337	-4.952	1.00	0.00	739	H20 PRO	62	-17.294
51	-10.771	-	6.433	-6.531	1.00	0.00	57	-10.518	614 C VAL	57	11.337	-4.952	1.00	0.00	740	H21 PRO	63	-17.294
52	-10.771	-	6.433	-6.531	1.00	0.00	58	-10.518	613 C VAL	58	11.337	-4.952	1.00	0.00	741	H22 PRO	64	-17.294
53	-10.771	-	6.433	-6.531	1.00	0.00	59	-10.518	612 C VAL	59	11.337	-4.952	1.00	0.00	742	H23 PRO	65	-17.294
54	-10.771	-	6.433	-6.531	1.00	0.00	60	-10.518	611 C VAL	60	11.337	-4.952	1.00	0.00	743	H24 PRO	66	-17.294
55	-10.771	-	6.433	-6.531	1.00	0.00	61	-10.518	610 C VAL	61	11.337	-4						

66	15.468	-	3.792	2.548	1.000	0.00	BID	ATOM	1193	HE1	LVS	71	12.561	4.642	3.049	1.000	0.00	BID	ATOM	1287	C	ALA	76	2.340
67	9.952	-	4.084	1.699	1.000	0.00	BID	ATOM	1194	HE2	LVS	71	14.267	4.601	1.147	1.000	0.00	BID	ATOM	1288	C	ALA	76	1.311
68	15.468	-	4.084	1.699	1.000	0.00	BID	ATOM	1195	HE1	LVS	71	14.267	4.601	1.147	1.000	0.00	BID	ATOM	1289	C	ALA	76	1.311
69	15.468	-	4.084	1.699	1.000	0.00	BID	ATOM	1196	HE2	LVS	71	14.267	4.601	1.147	1.000	0.00	BID	ATOM	1290	C	ALA	76	1.311
70	15.468	-	4.084	1.699	1.000	0.00	BID	ATOM	1197	HE1	LVS	71	14.267	4.601	1.147	1.000	0.00	BID	ATOM	1291	C	ALA	76	1.311
71	15.468	-	4.084	1.699	1.000	0.00	BID	ATOM	1198	HE2	LVS	71	14.267	4.601	1.147	1.000	0.00	BID	ATOM	1292	C	ALA	76	1.311
72	15.468	-	4.084	1.699	1.000	0.00	BID	ATOM	1199	HE1	LVS	71	14.267	4.601	1.147	1.000	0.00	BID	ATOM	1293	C	ALA	76	1.311
73	15.468	-	4.084	1.699	1.000	0.00	BID	ATOM	1200	HE2	LVS	71	14.267	4.601	1.147	1.000	0.00	BID	ATOM	1294	C	ALA	76	1.311
74	15.468	-	4.084	1.699	1.000	0.00	BID	ATOM	1201	HE1	LVS	71	14.267	4.601	1.147	1.000	0.00	BID	ATOM	1295	C	ALA	76	1.311
75	15.468	-	4.084	1.699	1.000	0.00	BID	ATOM	1202	HE2	LVS	71	14.267	4.601	1.147	1.000	0.00	BID	ATOM	1296	C	ALA	76	1.311
76	15.468	-	4.084	1.699	1.000	0.00	BID	ATOM	1203	HE1	LVS	71	14.267	4.601	1.147	1.000	0.00	BID	ATOM	1297	C	ALA	76	1.311
77	15.468	-	4.084	1.699	1.000	0.00	BID	ATOM	1204	HE2	LVS	71	14.267	4.601	1.147	1.000	0.00	BID	ATOM	1298	C	ALA	76	1.311
78	15.468	-	4.084	1.699	1.000	0.00	BID	ATOM	1205	HE1	LVS	71	14.267	4.601	1.147	1.000	0.00	BID	ATOM	1299	C	ALA	76	1.311
79	15.468	-	4.084	1.699	1.000	0.00	BID	ATOM	1206	HE2	LVS	71	14.267	4.601	1.147	1.000	0.00	BID	ATOM	1300	C	ALA	76	1.311
80	15.468	-	4.084	1.699	1.000	0.00	BID	ATOM	1207	HE1	LVS	71	14.267	4.601	1.147	1.000	0.00	BID	ATOM	1301	C	ALA	76	1.311
81	15.468	-	4.084	1.699	1.000	0.00	BID	ATOM	1208	HE2	LVS	71	14.267	4.601	1.147	1.000	0.00	BID	ATOM	1302	C	ALA	76	1.311
82	15.468	-	4.084	1.699	1.000	0.00	BID	ATOM	1209	HE1	LVS	71	14.267	4.601	1.147	1.000	0.00	BID	ATOM	1303	C	ALA	76	1.311
83	15.468	-	4.084	1.699	1.000	0.00	BID	ATOM	1210	HE2	LVS	71	14.267	4.601	1.147	1.000	0.00	BID	ATOM	1304	C	ALA	76	1.311
84	15.468	-	4.084	1.699	1.000	0.00	BID	ATOM	1211	HE1	LVS	71	14.267	4.601	1.147	1.000	0.00	BID	ATOM	1305	C	ALA	76	1.311
85	15.468	-	4.084	1.699	1.000	0.00	BID	ATOM	1212	HE2	LVS	71	14.267	4.601	1.147	1.000	0.00	BID	ATOM	1306	C			

UNITED STATES GOVERNMENT
OFFICE OF THE SECRETARY OF DEFENSE
WASHINGTON, D. C. 20301-4000

4.534 5.217 1.00 0.00 BFD ATOM 1945 C01 L1E 116 4.662
0.615 6.373 1.00 0.00 BFD ATOM 1946 H01 L1E 116 3.870
0.073 5.875 1.00 0.00 BFD ATOM 1947 H01 L1E 116 4.240
0.046 6.812 1.00 0.00 BFD ATOM 1948 H01 L1E 116 3.148
1.751 8.053 1.00 0.00 BFD ATOM 1949 C 11E 116 6.032
0.944 8.154 1.00 0.00 BFD ATOM 1951 N ASP 117 7.024
2.465 9.014 1.00 0.00 BFD ATOM 1952 H01 ASP 117 6.222
3.424 8.974 1.00 0.00 BFD ATOM 1953 C01 ASP 117 5.079
1.462 10.275 1.00 0.00 BFD ATOM 1954 H01 ASP 117 5.605
1.462 10.275 1.00 0.00 BFD ATOM 1955 H01 ASP 117 5.197
0.409 10.013 1.00 0.00 BFD ATOM 1956 H01 ASP 117 5.148
0.247 10.202 1.00 0.00 BFD ATOM 1957 H02 ASP 117 4.664
0.596 8.976 1.00 0.00 BFD ATOM 1958 C01 ASP 117 3.722
0.555 10.176 1.00 0.00 BFD ATOM 1959 C01 ASP 117 2.977
1.488 10.787 1.00 0.00 BFD ATOM 1960 C02 ASP 117 1.572
1.488 10.787 1.00 0.00 BFD ATOM 1961 C ASP 117 7.044
1.504 11.154 1.00 0.00 BFD ATOM 1962 N ASP 117 6.144
0.892 12.209 1.00 0.00 BFD ATOM 1963 N LVS 118 8.206
1.897 10.725 1.00 0.00 BFD ATOM 1964 H01 LVS 118 8.242
2.384 9.179 1.00 0.00 BFD ATOM 1965 C01 LVS 118 9.116
1.613 11.488 1.00 0.00 BFD ATOM 1966 H01 LVS 118 10.248
1.613 11.488 1.00 0.00 BFD ATOM 1967 C01 LVS 118 9.215
2.212 11.989 1.00 0.00 BFD ATOM 1968 H01 LVS 118 10.248
1.624 13.400 1.00 0.00 BFD ATOM 1969 H02 LVS 118 10.292
2.199 13.149 1.00 0.00 BFD ATOM 1970 C01 LVS 118 8.118
3.656 12.495 1.00 0.00 BFD ATOM 1971 H01 LVS 118 7.921
3.719 12.296 1.00 0.00 BFD ATOM 1972 H02 LVS 118 8.595
2.846 12.121 1.00 0.00 BFD ATOM 1973 C01 LVS 118 9.457
2.846 12.121 1.00 0.00 BFD ATOM 1974 H01 LVS 118 10.488
4.873 12.133 1.00 0.00 BFD ATOM 1975 H02 LVS 118 9.208
4.078 11.613 1.00 0.00 BFD ATOM 1976 C01 LVS 118 8.502
5.794 11.411 1.00 0.00 BFD ATOM 1977 H01 LVS 118 8.487
5.425 10.902 1.00 0.00 BFD ATOM 1978 H02 LVS 118 10.212
6.386 12.469 1.00 0.00 BFD ATOM 1979 H01 LVS 118 11.483
6.452 10.743 1.00 0.00 BFD ATOM 1980 H01 LVS 118 10.206
7.656 11.096 1.00 0.00 BFD ATOM 1982 H02 LVS 118 9.457
6.459 9.921 1.00 0.00 BFD ATOM 1983 C LVS 118 9.047
0.110 11.591 1.00 0.00 BFD ATOM 1984 OT1 LVS 118 10.454
0.441 10.602 1.00 0.00 BFD ATOM 1985 OT2 LVS 118 10.454
0.302 13.459 1.00 0.00 BFD END

ATOM	1455	CE2	PHE	74	7.085	-2.476	3.082	1.00	0.00	PROT	1522	HA	GLN	79	1.775	2.673	-3.870	1.00	0.00	PROT
ATOM	1456	HE2	PHE	74	6.724	-3.203	3.795	1.00	0.00	PROT	1523	CB	GLN	79	3.106	1.772	-5.312	1.00	0.00	PROT
ATOM	1457	CZ	PHE	74	6.901	-1.109	3.322	1.00	0.00	PROT	1524	HB1	GLN	79	4.000	2.185	-4.869	1.00	0.00	PROT
ATOM	1458	HZ	PHE	74	6.401	-0.781	4.220	1.00	0.00	PROT	1525	HE2	GLN	79	3.316	0.783	-5.691	1.00	0.00	PROT
ATOM	1459	C	PHE	74	7.138	-1.943	1.958	1.00	0.00	PROT	1526	CG	GLN	79	2.642	2.670	-6.461	1.00	0.00	PROT
ATOM	1460	N	PHE	74	5.930	-1.839	1.885	1.00	0.00	PROT	1527	HG1	GLN	79	3.421	2.734	-7.206	1.00	0.00	PROT
ATOM	1461	O	PHE	75	7.852	-1.106	-2.654	1.00	0.00	PROT	1528	HG2	GLN	79	1.751	2.252	-6.907	1.00	0.00	PROT
ATOM	1462	HN	MET	75	8.826	-1.209	-2.689	1.00	0.00	PROT	1529	CD	GLN	79	2.334	4.070	-5.923	1.00	0.00	PROT
ATOM	1463	CA	MET	75	7.200	0.006	-3.397	1.00	0.00	PROT	1530	OE1	GLN	79	2.300	4.920	-5.878	1.00	0.00	PROT
ATOM	1464	HA	MET	75	6.821	0.746	-2.708	1.00	0.00	PROT	1531	NE2	GLN	79	1.126	4.346	-5.510	1.00	0.00	PROT
ATOM	1465	CB	MET	75	8.324	0.604	-4.242	1.00	0.00	PROT	1532	HE21	GLN	79	0.427	3.660	-5.546	1.00	0.00	PROT
ATOM	1466	HB1	MET	75	7.921	1.351	-4.906	1.00	0.00	PROT	1533	HE22	GLN	79	0.919	5.239	-5.164	1.00	0.00	PROT
ATOM	1467	HE2	MET	75	8.792	-0.169	-4.821	1.00	0.00	PROT	1534	C	GLN	79	0.751	1.040	-4.840	1.00	0.00	PROT
ATOM	1468	CG	MET	75	9.365	1.235	3.316	1.00	0.00	PROT	1535	O	GLN	79	-0.188	1.707	-5.223	1.00	0.00	PROT
ATOM	1469	HG1	MET	75	9.058	1.110	-2.289	1.00	0.00	PROT	1536	N	ARG	80	0.722	-0.266	-4.886	1.00	0.00	PROT
ATOM	1470	HG2	MET	75	10.312	0.757	-3.466	1.00	0.00	PROT	1537	HN	ARG	80	1.485	-0.785	-4.559	1.00	0.00	PROT
ATOM	1471	SD	MET	75	9.512	2.993	-3.689	1.00	0.00	PROT	1538	CA	ARG	80	-0.480	-0.962	-5.420	1.00	0.00	PROT
ATOM	1472	CE	MET	75	7.867	3.463	-3.126	1.00	0.00	PROT	1539	HA	ARG	80	-0.746	-0.558	-6.383	1.00	0.00	PROT
ATOM	1473	HE1	MET	75	7.927	3.799	-2.102	1.00	0.00	PROT	1540	CB	ARG	80	-0.074	-2.432	-5.547	1.00	0.00	PROT
ATOM	1474	HE2	MET	75	7.209	2.609	-3.189	1.00	0.00	PROT	1541	HB1	ARG	80	0.739	-2.639	-4.868	1.00	0.00	PROT
ATOM	1475	HE3	MET	75	7.490	4.261	-3.751	1.00	0.00	PROT	1542	HB2	ARG	80	-0.918	-3.059	-5.296	1.00	0.00	PROT
ATOM	1476	C	MET	75	6.068	-0.524	-4.282	1.00	0.00	PROT	1543	CG	ARG	80	0.373	-2.731	-6.984	1.00	0.00	PROT
ATOM	1477	O	MET	75	5.160	0.199	-4.639	1.00	0.00	PROT	1544	HG1	ARG	80	0.694	-3.759	-7.049	1.00	0.00	PROT
ATOM	1478	N	ALA	76	6.097	-1.786	-4.617	1.00	0.00	PROT	1545	HG2	ARG	80	1.197	-2.083	-7.244	1.00	0.00	PROT
ATOM	1479	HN	ALA	76	6.838	-2.356	-4.324	1.00	0.00	PROT	1546	CD	ARG	80	-0.785	-2.498	-7.968	1.00	0.00	PROT
ATOM	1480	CA	ALA	76	5.017	-2.351	-5.474	1.00	0.00	PROT	1547	HD1	ARG	80	-0.534	-2.896	-8.940	1.00	0.00	PROT
ATOM	1481	HA	ALA	76	4.859	-1.724	-6.339	1.00	0.00	PROT	1548	HD2	ARG	80	-1.008	-1.446	-8.043	1.00	0.00	PROT
ATOM	1482	CB	ALA	76	5.533	-3.725	-5.903	1.00	0.00	PROT	1549	NE	ARG	80	-1.951	-3.240	-7.395	1.00	0.00	PROT
ATOM	1483	HB1	ALA	76	4.696	-4.387	-6.072	1.00	0.00	PROT	1550	HE	ARG	80	-1.794	-3.974	-6.765	1.00	0.00	PROT
ATOM	1484	HB2	ALA	76	6.162	-4.133	-5.125	1.00	0.00	PROT	1551	C	ARG	80	-3.181	-2.927	-7.732	1.00	0.00	PROT
ATOM	1485	HB3	ALA	76	6.104	-3.627	-6.814	1.00	0.00	PROT	1552	NH1	ARG	80	-3.427	-1.954	-8.574	1.00	0.00	PROT
ATOM	1486	C	ALA	76	3.715	-2.502	-4.682	1.00	0.00	PROT	1553	NH11	ARG	80	-4.372	-1.732	-8.814	1.00	0.00	PROT
ATOM	1487	O	ALA	76	2.753	-1.798	-4.915	1.00	0.00	PROT	1554	NH12	ARG	80	-2.678	-1.433	-8.980	1.00	0.00	PROT
ATOM	1488	N	ASP	77	3.668	-3.429	-3.760	1.00	0.00	PROT	1555	NH2	ARG	80	-4.179	-3.592	-7.218	1.00	0.00	PROT
ATOM	1489	HN	ASP	77	4.449	-3.996	-3.597	1.00	0.00	PROT	1556	HH21	ARG	80	-5.117	-3.357	-6.574	1.00	0.00	PROT
ATOM	1490	CA	ASP	77	1.640	-4.028	-3.636	1.00	0.00	PROT	1557	HH22	ARG	80	-4.004	-4.337	-7.570	1.00	0.00	PROT
ATOM	1491	HA	ASP	77	2.766	-4.897	-1.923	1.00	0.00	PROT	1558	C	ARG	80	-1.649	-0.820	-4.445	1.00	0.00	PROT
ATOM	1492	CB	ASP	77	1.930	-4.828	-1.205	1.00	0.00	PROT	1559	O	ARG	80	-2.784	-1.067	-4.792	1.00	0.00	PROT
ATOM	1493	HB1	ASP	77	2.986	-5.636	-2.409	1.00	0.00	PROT	1560	N	VAL	81	-1.381	-0.472	-3.213	1.00	0.00	PROT
ATOM	1494	HB2	ASP	77	3.986	-4.245	-1.121	1.00	0.00	PROT	1561	HN	VAL	81	-0.468	-0.226	-2.958	1.00	0.00	PROT
ATOM	1495	CG	ASP	77	3.851	-4.078	0.080	1.00	0.00	PROT	1562	CA	VAL	81	-2.497	-0.266	-2.253	1.00	0.00	PROT
ATOM	1496	OD1	ASP	77	5.034	-4.080	-1.718	1.00	0.00	PROT	1563	HA	VAL	81	-3.256	-1.024	-2.380	1.00	0.00	PROT
ATOM	1497	OD2	ASP	77	1.944	-2.345	-2.337	1.00	0.00	PROT	1564	CB	VAL	81	-1.866	-0.359	-0.857	1.00	0.00	PROT
ATOM	1498	C	ASP	77	0.781	-1.993	-2.389	1.00	0.00	PROT	1565	HB	VAL	81	-0.983	0.264	-0.570	1.00	0.00	PROT
ATOM	1499	O	ASP	77	2.830	-1.621	-1.700	1.00	0.00	PROT	1566	CG1	VAL	81	-1.480	-1.810	-1.490	1.00	0.00	PROT
ATOM	1500	N	LEU	78	3.766	-1.906	-1.667	1.00	0.00	PROT	1567	HG11	VAL	81	-1.187	-2.293	-1.490	1.00	0.00	PROT
ATOM	1501	HN	LEU	78	2.415	-0.345	-1.057	1.00	0.00	PROT	1568	HG12	VAL	81	-2.326	-2.329	-0.144	1.00	0.00	PROT
ATOM	1502	CB	LEU	78	1.688	-0.536	-0.282	1.00	0.00	PROT	1569	HG13	VAL	81	-0.655	-1.832	0.129	1.00	0.00	PROT
ATOM	1503	HA	LEU	78	3.705	0.226	-0.455	1.00	0.00	PROT	1570	CG2	VAL	81	-2.872	0.112	0.201	1.00	0.00	PROT
ATOM	1504	CB	LEU	78	4.265	-0.572	0.010	1.00	0.00	PROT	1571	HG21	VAL	81	-3.713	-0.565	0.223	1.00	0.00	PROT
ATOM	1505	HB1	LEU	78	4.299	0.671	-0.219	1.00	0.00	PROT	1572	HG22	VAL	81	-3.217	1.106	-0.046	1.00	0.00	PROT
ATOM	1506	HB2	LEU	78	3.370	1.291	0.596	1.00	0.00	PROT	1573	HG23	VAL	81	-2.396	0.126	1.170	1.00	0.00	PROT
ATOM	1507	CG	LEU	78	2.897	2.134	0.116	1.00	0.00	PROT	1574	C	VAL	81	-3.071	1.119	-2.498	1.00	0.00	PROT
ATOM	1508	HG	LEU	78	4.661	1.751	1.277	1.00	0.00	PROT	1575	O	VAL	81	-4.262	1.338	-2.448	1.00	0.00	PROT
ATOM	1509	CD1	LEU	78	5.445	1.842	0.541	1.00	0.00	PROT	1576	N	PHE	82	-2.211	2.052	-2.777	1.00	0.00	PROT
ATOM	1510	HD11	LEU	78	4.951	1.027	2.025	1.00	0.00	PROT	1577	HN	PHE	82	-2.256	1.830	-2.832	1.00	0.00	PROT
ATOM	1511	HD12	LEU	78	4.497	2.709	1.749	1.00	0.00	PROT	1578	CA	PHE	82	-2.670	3.430	-3.074	1.00	0.00	PROT
ATOM	1512	HD13	LEU	78	2.427	0.708	1.653	1.00	0.00	PROT	1579	HB	PHE	82	-3.460	3.724	-2.398	1.00	0.00	PROT
ATOM	1513	CD2	LEU	78	2.801	0.942	2.638	1.00	0.00	PROT	1580	HA	PHE	82	-1.430	4.302	-2.869	1.00	0.00	PROT
ATOM	1514	HD21	LEU	78	2.373	-0.364	1.534	1.00	0.00	PROT	1581	HB1	PHE	82	-0.651	4.048	-3.609	1.00	0.00	PROT
ATOM	1515	HD22	LEU	78	1.442	1.134	1.530	1.00	0.00	PROT	1582	HE2	PHE	82	-1.702	5.331	-2.983	1.00	0.00	PROT
ATOM	1516	HD23	LEU	78	1.834	0.598	-2.112	1.00	0.00	PROT	1583	CG	PHE	82	-0.850	4.088	-1.486	1.00	0.00	PROT
ATOM	1517	C	LEU	78	0.727	1.090	-1.981	1.00	0.00	PROT	1584	CD1	PHE	82	0.538	4.105	-1.307	1.00	0.00	PROT
ATOM	1518	O	LEU	78	2.550	0.823	-3.180	1.00	0.00	PROT	1585	HD1	PHE	82	1.190	4.259	-2.154	1.00	0.00	PROT
ATOM	1519	N	GLN	79	3.427	0.397	-3.285	1.00	0.00	PROT	1586	CD2	PHE	82	-1.695	3.896	-0.384	1.00	0.00	PROT
ATOM	1520	HN	GLN	79	2.003	1.691	-4.256	1.00	0.00	PROT	1587	HD2	PHE	82	-2.766	3.886	-0.520	1.00	0.00	PROT
ATOM	1521	CA	GLN	79	7.085	-2.476	3.082	1.00	0.00	PROT	1588	CE1	PHE	82	1.083	3.916	-0.032	1.00	0.00	PROT

ATOM	1589	HE1 PHE	82	2.154	3.925	0.105	1.00	0.00	PROT	1556	O	LYS	86	-8.543	5.924	-8.012	1.00	0.00	PROT
ATOM	1590	CE2 PHE	82	-1.148	3.705	0.891	1.00	0.00	PROT	1557	N	GLU	87	-7.671	3.924	-7.734	1.00	0.00	PROT
ATOM	1591	HE2 PHE	82	-1.797	3.551	1.739	1.00	0.00	PROT	1558	HN	GLU	87	-7.112	3.329	-7.192	1.00	0.00	PROT
ATOM	1592	CZ PHE	82	0.240	3.716	1.067	1.00	0.00	PROT	1559	CA	GLU	87	-8.305	3.412	-8.981	1.00	0.00	PROT
ATOM	1593	HZ PHE	82	0.661	3.569	2.051	1.00	0.00	PROT	1560	HA	GLU	87	-7.975	3.985	-9.836	1.00	0.00	PROT
ATOM	1594	C PHE	82	-3.139	3.510	-4.526	1.00	0.00	PROT	1561	CB	GLU	87	-7.819	1.964	-9.088	1.00	0.00	PROT
ATOM	1595	O PHE	82	-4.149	4.111	-4.835	1.00	0.00	PROT	1562	HB1	GLU	87	-6.936	1.836	-8.480	1.00	0.00	PROT
ATOM	1596	N THR	83	-2.407	2.900	-5.419	1.00	0.00	PROT	1563	HB2	GLU	87	-8.594	1.295	-8.740	1.00	0.00	PROT
ATOM	1597	HN THR	83	-1.599	2.420	-5.141	1.00	0.00	PROT	1564	CG	GLU	87	-7.780	2.463	-11.176	1.00	0.00	PROT
ATOM	1598	CA THR	83	-2.798	2.923	-6.855	1.00	0.00	PROT	1565	HG1	GLU	87	-7.480	1.638	-10.544	1.00	0.00	PROT
ATOM	1599	HA THR	83	-2.812	3.938	-7.224	1.00	0.00	PROT	1566	HG2	GLU	87	-8.016	0.747	-10.843	1.00	0.00	PROT
ATOM	1600	CB THR	83	-1.711	2.111	-7.564	1.00	0.00	PROT	1567	CD	GLU	87	-5.980	1.403	-10.680	1.00	0.00	PROT
ATOM	1601	HB THR	83	-1.671	1.118	-7.142	1.00	0.00	PROT	1568	OE1	GLU	87	-5.228	2.317	-10.382	1.00	0.00	PROT
ATOM	1602	OG1 THR	83	-0.455	2.751	-7.391	1.00	0.00	PROT	1569	OE2	GLU	87	-5.604	0.312	-11.074	1.00	0.00	PROT
ATOM	1603	HG1 THR	83	-0.446	3.541	-7.936	1.00	0.00	PROT	1570	C	GLU	87	-9.831	3.452	-8.864	1.00	0.00	PROT
ATOM	1604	CG2 THR	83	-2.029	2.019	-9.057	1.00	0.00	PROT	1571	O	GLU	87	-10.529	3.767	-9.807	1.00	0.00	PROT
ATOM	1605	HG21 THR	83	-1.107	1.973	-9.618	1.00	0.00	PROT	1572	N	TYR	88	-10.352	3.133	-7.711	1.00	0.00	PROT
ATOM	1606	HG22 THR	83	-2.592	2.889	-9.359	1.00	0.00	PROT	1573	HN	TYR	88	-9.768	2.870	-6.970	1.00	0.00	PROT
ATOM	1607	HG23 THR	83	-2.611	1.129	-9.246	1.00	0.00	PROT	1574	CA	TYR	88	-11.833	3.129	-7.530	1.00	0.00	PROT
ATOM	1608	C THR	83	-4.166	2.267	-7.040	1.00	0.00	PROT	1575	HA	TYR	88	-12.324	3.399	-8.453	1.00	0.00	PROT
ATOM	1609	O THR	83	-5.064	2.842	-7.623	1.00	0.00	PROT	1576	CB	TYR	88	-12.153	1.671	-7.162	1.00	0.00	PROT
ATOM	1610	N ASN	84	-4.341	1.070	-6.545	1.00	0.00	PROT	1577	HB1	TYR	88	-12.049	1.052	-8.041	1.00	0.00	PROT
ATOM	1611	HN ASN	84	-3.612	0.620	-6.070	1.00	0.00	PROT	1578	HB2	TYR	88	-11.460	1.335	-6.405	1.00	0.00	PROT
ATOM	1612	CA ASN	84	-5.666	0.405	-6.690	1.00	0.00	PROT	1579	CG	TYR	88	-13.564	1.553	-6.634	1.00	0.00	PROT
ATOM	1613	HA ASN	84	-5.929	0.343	-7.735	1.00	0.00	PROT	1580	CD1	TYR	88	-14.640	2.046	-7.380	1.00	0.00	PROT
ATOM	1614	CB ASN	84	-5.475	-1.020	-6.114	1.00	0.00	PROT	1581	HD1	TYR	88	-14.465	2.512	-8.339	1.00	0.00	PROT
ATOM	1615	HB1 ASN	84	-6.068	-1.713	-6.697	1.00	0.00	PROT	1582	CD2	TYR	88	-13.790	0.950	-5.392	1.00	0.00	PROT
ATOM	1616	HB2 ASN	84	-4.432	-1.291	-6.193	1.00	0.00	PROT	1583	HD2	TYR	88	-12.958	0.571	-4.817	1.00	0.00	PROT
ATOM	1617	CG ASN	84	-5.902	-1.115	-4.636	1.00	0.00	PROT	1584	CE1	TYR	88	-15.944	1.934	-6.883	1.00	0.00	PROT
ATOM	1618	OD1 ASN	84	-7.044	-0.865	-4.304	1.00	0.00	PROT	1585	HE1	TYR	88	-16.775	2.313	-7.459	1.00	0.00	PROT
ATOM	1619	ND2 ASN	84	-5.032	-1.484	-3.739	1.00	0.00	PROT	1586	CE2	TYR	88	-15.091	0.840	-4.895	1.00	0.00	PROT
ATOM	1620	HD21 ASN	84	-5.296	-1.548	-2.797	1.00	0.00	PROT	1587	HE2	TYR	88	-15.262	0.372	-3.939	1.00	0.00	PROT
ATOM	1621	HD22 ASN	84	-4.111	-1.689	-4.004	1.00	0.00	PROT	1588	CZ	TYR	88	-16.170	1.330	-5.640	1.00	0.00	PROT
ATOM	1622	C ASN	84	-6.725	1.219	-5.938	1.00	0.00	PROT	1589	OH	TYR	88	-17.455	1.219	-5.149	1.00	0.00	PROT
ATOM	1623	O ASN	84	-7.789	1.500	-6.452	1.00	0.00	PROT	1590	HH	TYR	88	-18.049	1.106	-5.895	1.00	0.00	PROT
ATOM	1624	N CYS	85	-6.429	1.616	-4.727	1.00	0.00	PROT	1591	C	TYR	88	-12.244	4.092	-6.402	1.00	0.00	PROT
ATOM	1625	HN CYS	85	-5.558	1.390	-4.333	1.00	0.00	PROT	1592	O	TYR	88	-13.395	4.460	-6.280	1.00	0.00	PROT
ATOM	1626	CA CYS	85	-7.407	2.437	-3.960	1.00	0.00	PROT	1593	N ASN	89	-11.311	4.498	-5.582	1.00	0.00	PROT	
ATOM	1627	HA CYS	85	-8.278	1.850	-3.710	1.00	0.00	PROT	1594	HN ASN	89	-10.393	4.178	-5.695	1.00	0.00	PROT	
ATOM	1628	CB CYS	85	-6.667	2.863	-2.642	1.00	0.00	PROT	1595	CA ASN	89	-11.633	5.425	-4.454	1.00	0.00	PROT	
ATOM	1629	HB1 CYS	85	-7.062	3.805	-2.340	1.00	0.00	PROT	1596	HA ASN	89	-12.102	4.887	-3.643	1.00	0.00	PROT	
ATOM	1630	HB2 CYS	85	-5.615	2.973	-2.906	1.00	0.00	PROT	1597	CB ASN	89	-10.276	5.982	-4.013	1.00	0.00	PROT	
ATOM	1631	SG CYS	85	-6.897	1.605	-1.409	1.00	0.00	PROT	1598	HB1 ASN	89	-9.588	5.946	-4.843	1.00	0.00	PROT	
ATOM	1632	HG CYS	85	-6.090	1.088	-4.787	1.00	0.00	PROT	1599	HB2 ASN	89	-10.397	7.007	-3.695	1.00	0.00	PROT	
ATOM	1633	C CYS	85	-7.804	3.659	-4.787	1.00	0.00	PROT	1600	CG ASN	89	-9.715	5.156	-2.852	1.00	0.00	PROT	
ATOM	1634	O CYS	85	-8.959	3.871	-5.072	1.00	0.00	PROT	1601	OD1 ASN	89	-8.962	5.662	-2.045	1.00	0.00	PROT	
ATOM	1635	N LYS	86	-6.847	4.433	-5.219	1.00	0.00	PROT	1602	ND2 ASN	89	-10.032	3.896	-2.740	1.00	0.00	PROT	
ATOM	1636	HN LYS	86	-5.915	4.232	-4.996	1.00	0.00	PROT	1603	HD21 ASN	89	-9.667	3.366	-2.001	1.00	0.00	PROT	
ATOM	1637	CA LYS	86	-7.174	5.616	-6.064	1.00	0.00	PROT	1604	HD22 ASN	89	-10.635	3.481	-3.391	1.00	0.00	PROT	
ATOM	1638	HA LYS	86	-7.808	6.303	-5.524	1.00	0.00	PROT	1605	C ASN	89	-12.527	6.579	-4.921	1.00	0.00	PROT	
ATOM	1639	CB LYS	86	-5.823	6.263	-6.367	1.00	0.00	PROT	1606	O ASN	89	-12.553	6.904	-6.091	1.00	0.00	PROT	
ATOM	1640	HB1 LYS	86	-5.174	5.538	-6.837	1.00	0.00	PROT	1607	N PRO	90	-13.220	7.179	-3.983	1.00	0.00	PROT	
ATOM	1641	HB2 LYS	86	-5.966	7.102	-7.031	1.00	0.00	PROT	1608	CA PRO	90	-14.089	8.334	-4.311	1.00	0.00	PROT	
ATOM	1642	CG LYS	86	-5.189	6.745	-5.062	1.00	0.00	PROT	1609	HA PRO	90	-14.903	8.033	-4.943	1.00	0.00	PROT	
ATOM	1643	HG1 LYS	86	-5.557	6.147	-4.241	1.00	0.00	PROT	1610	CB PRO	90	-14.615	8.801	-2.954	1.00	0.00	PROT	
ATOM	1644	HG2 LYS	86	-4.115	6.647	-5.125	1.00	0.00	PROT	1611	HB1 PRO	90	-14.055	9.655	-2.612	1.00	0.00	PROT	
ATOM	1645	CD LYS	86	-5.557	8.212	-4.829	1.00	0.00	PROT	1612	HB2 PRO	90	-15.664	9.044	-3.023	1.00	0.00	PROT	
ATOM	1646	HD1 LYS	86	-6.383	8.270	-4.136	1.00	0.00	PROT	1613	CG PRO	90	-14.411	7.644	-2.028	1.00	0.00	PROT	
ATOM	1647	HD2 LYS	86	-5.841	8.665	-5.767	1.00	0.00	PROT	1614	HG1 PRO	90	-14.206	8.003	-1.031	1.00	0.00	PROT	
ATOM	1648	CE LYS	86	-4.351	8.953	-4.250	1.00	0.00	PROT	1615	HG2 PRO	90	-15.291	7.018	-2.022	1.00	0.00	PROT	
ATOM	1649	HE1 LYS	86	-3.952	9.477	-4.050	1.00	0.00	PROT	1616	CD PRO	90	-13.233	6.870	-2.547	1.00	0.00	PROT	
ATOM	1650	HE2 LYS	86	-4.630	9.477	-3.347	1.00	0.00	PROT	1617	HD2 PRO	90	-13.375	5.811	-2.388	1.00	0.00	PROT	
ATOM	1651	NZ LYS	86	-3.914	10.313	-6.287	1.00	0.00	PROT	1618	HD1 PRO	90	-12.320	7.207	-2.				

ATOM	1723	HA	PRO	91	-12.548	11.189	-6.949	1.00	0.00	PROT	1790	CE2	TYR	95	-11.373	2.208	1.139	1.00	0.00	PROT
ATOM	1724	CB	PRO	91	-14.298	12.444	-6.713	1.00	0.00	PROT	1791	CE2	TYR	95	-10.638	1.438	0.954	1.00	0.00	PROT
ATOM	1725	HB1	PRO	91	-14.390	13.335	-6.110	1.00	0.00	PROT	1792	CE2	TYR	95	-12.394	1.992	2.071	1.00	0.00	PROT
ATOM	1726	HB2	PRO	91	-14.083	12.709	-7.738	1.00	0.00	PROT	1793	OH	TYR	95	-12.461	0.796	2.755	1.00	0.00	PROT
ATOM	1727	CG	PRO	91	-15.561	11.638	-6.642	1.00	0.00	PROT	1794	HH	TYR	95	-11.566	0.536	2.985	1.00	0.00	PROT
ATOM	1728	HG1	PRO	91	-15.740	11.151	-7.589	1.00	0.00	PROT	1795	C	TYR	95	-10.263	7.359	-0.058	1.00	0.00	PROT
ATOM	1729	HG2	PRO	91	-16.394	12.279	-6.394	1.00	0.00	PROT	1796	O	TYR	95	-9.128	6.931	0.009	1.00	0.00	PROT
ATOM	1730	CD	PRO	91	-15.372	10.606	-5.565	1.00	0.00	PROT	1797	N	TYR	96	-10.562	8.375	-0.818	1.00	0.00	PROT
ATOM	1731	HD2	PRO	91	-15.870	9.685	-5.829	1.00	0.00	PROT	1798	NN	TYR	96	-11.485	8.704	-0.854	1.00	0.00	PROT
ATOM	1732	HD1	PRO	91	-15.731	10.976	-4.616	1.00	0.00	PROT	1799	CA	TYR	96	-9.511	9.020	-1.652	1.00	0.00	PROT
ATOM	1733	C	PRO	91	-12.386	12.274	-5.276	1.00	0.00	PROT	1800	HA	TYR	96	-8.931	8.273	-2.171	1.00	0.00	PROT
ATOM	1734	O	PRO	91	-11.242	12.636	-3.940	1.00	0.00	PROT	1801	CB	TYR	96	-10.287	9.877	-2.650	1.00	0.00	PROT
ATOM	1735	NN	GLJ	92	-12.984	12.463	-3.819	1.00	0.00	PROT	1802	HB1	TYR	96	-10.677	10.750	-2.148	1.00	0.00	PROT
ATOM	1736	HN	GLJ	92	-13.902	12.142	-2.805	1.00	0.00	PROT	1803	HB2	TYR	96	-11.103	9.301	-3.054	1.00	0.00	PROT
ATOM	1737	CA	GLJ	92	-12.291	13.137	-2.805	1.00	0.00	PROT	1804	CG	TYR	96	-9.365	10.308	-3.766	1.00	0.00	PROT
ATOM	1738	HA	GLJ	92	-11.390	12.603	-2.540	1.00	0.00	PROT	1805	CD1	TYR	96	-8.796	11.587	-3.747	1.00	0.00	PROT
ATOM	1739	CB	GLJ	92	-11.956	14.546	-3.302	1.00	0.00	PROT	1806	HD1	TYR	96	-9.018	12.265	-2.937	1.00	0.00	PROT
ATOM	1740	HB1	GLJ	92	-12.754	15.222	-3.033	1.00	0.00	PROT	1807	CD2	TYR	96	-9.077	9.428	-4.816	1.00	0.00	PROT
ATOM	1741	HB2	GLJ	92	-11.841	14.534	-4.375	1.00	0.00	PROT	1808	HD2	TYR	96	-9.515	8.441	-4.830	1.00	0.00	PROT
ATOM	1742	CG	GLJ	92	-10.650	15.014	-2.653	1.00	0.00	PROT	1809	CE1	TYR	96	-7.940	11.987	-4.780	1.00	0.00	PROT
ATOM	1743	HG1	GLJ	92	-9.920	15.220	-3.422	1.00	0.00	PROT	1810	CE1	TYR	96	-7.502	12.974	-6.519	1.00	0.00	PROT
ATOM	1744	HG2	GLJ	92	-10.274	14.240	-1.998	1.00	0.00	PROT	1811	CE2	TYR	96	-7.999	9.151	-5.849	1.00	0.00	PROT
ATOM	1745	CD	GLJ	92	-10.910	16.285	-1.843	1.00	0.00	PROT	1812	CE2	TYR	96	-7.652	11.108	-5.831	1.00	0.00	PROT
ATOM	1746	OE1	GLJ	92	-10.924	17.350	-2.437	1.00	0.00	PROT	1813	CE2	TYR	96	-6.808	11.503	-6.850	1.00	0.00	PROT
ATOM	1747	OE2	GLJ	92	-11.089	16.172	-0.641	1.00	0.00	PROT	1814	HH	TYR	96	-6.254	12.213	-6.519	1.00	0.00	PROT
ATOM	1748	C	GLJ	92	-13.247	13.203	-1.615	1.00	0.00	PROT	1815	HH	TYR	96	-8.603	9.905	-0.798	1.00	0.00	PROT
ATOM	1749	O	GLJ	92	-13.531	14.259	-1.087	1.00	0.00	PROT	1816	C	TYR	96	-7.535	10.294	-1.220	1.00	0.00	PROT
ATOM	1750	NN	SR	93	-13.786	12.079	-1.225	1.00	0.00	PROT	1817	O	TYR	96	-9.023	10.241	0.390	1.00	0.00	PROT
ATOM	1751	HN	SR	93	-13.554	11.245	-1.680	1.00	0.00	PROT	1818	N	LVS	97	-9.895	9.929	0.709	1.00	0.00	PROT
ATOM	1752	CA	SR	93	-14.767	12.067	-0.106	1.00	0.00	PROT	1819	HN	LVS	97	-8.186	11.122	1.253	1.00	0.00	PROT
ATOM	1753	HA	SR	93	-15.148	13.059	0.067	1.00	0.00	PROT	1820	CA	LVS	97	-7.766	11.928	0.669	1.00	0.00	PROT
ATOM	1754	CB	SR	93	-15.893	11.146	-0.584	1.00	0.00	PROT	1821	HA	LVS	97	-9.156	11.675	2.300	1.00	0.00	PROT
ATOM	1755	HB1	SR	93	-16.602	10.116	-0.438	1.00	0.00	PROT	1822	CB	LVS	97	-9.527	10.864	2.910	1.00	0.00	PROT
ATOM	1756	HB2	SR	93	-16.081	11.322	-1.632	1.00	0.00	PROT	1823	HB1	LVS	97	-8.641	12.388	2.926	1.00	0.00	PROT
ATOM	1757	OG	SR	93	-17.072	11.414	0.161	1.00	0.00	PROT	1824	HB2	LVS	97	-10.330	12.364	1.599	1.00	0.00	PROT
ATOM	1758	HG	SR	93	-17.698	10.707	-0.011	1.00	0.00	PROT	1825	CG	LVS	97	-11.167	11.683	1.545	1.00	0.00	PROT
ATOM	1759	C	SR	93	-14.138	11.515	1.470	1.00	0.00	PROT	1826	HG1	LVS	97	-10.034	12.652	0.602	1.00	0.00	PROT
ATOM	1760	N	GLJ	94	-14.011	12.212	2.157	1.00	0.00	PROT	1827	HG2	LVS	97	-10.735	13.609	2.391	1.00	0.00	PROT
ATOM	1761	N	GLJ	94	-13.765	10.264	1.176	1.00	0.00	PROT	1828	CD	LVS	97	-11.605	14.058	1.936	1.00	0.00	PROT
ATOM	1762	NN	GLJ	94	-13.882	9.706	0.370	1.00	0.00	PROT	1829	HD1	LVS	97	-10.965	13.329	3.408	1.00	0.00	PROT
ATOM	1763	CA	GLJ	94	-13.170	9.689	2.417	1.00	0.00	PROT	1830	HD2	LVS	97	-9.581	14.613	2.387	1.00	0.00	PROT
ATOM	1764	HA	GLJ	94	-12.742	10.472	3.022	1.00	0.00	PROT	1831	CE	LVS	97	-8.897	14.402	3.195	1.00	0.00	PROT
ATOM	1765	CB	GLJ	94	-14.346	9.044	3.150	1.00	0.00	PROT	1832	HE1	LVS	97	-9.064	14.588	1.439	1.00	0.00	PROT
ATOM	1766	HB1	GLJ	94	-15.248	9.192	2.577	1.00	0.00	PROT	1833	HE2	LVS	97	-10.229	15.939	2.589	1.00	0.00	PROT
ATOM	1767	HB2	GLJ	94	-14.163	7.986	3.268	1.00	0.00	PROT	1834	NZ	LVS	97	-10.831	16.159	1.769	1.00	0.00	PROT
ATOM	1768	CG	GLJ	94	-14.506	9.692	4.527	1.00	0.00	PROT	1835	HA	CYS	98	-5.857	8.169	2.699	1.00	0.00	PROT
ATOM	1769	HG1	GLJ	94	-14.319	10.753	4.449	1.00	0.00	PROT	1836	HA	CYS	98	-8.045	8.604	1.675	1.00	0.00	PROT
ATOM	1770	HG2	GLJ	94	-15.511	9.529	4.888	1.00	0.00	PROT	1837	HZ1	LVS	97	-10.831	15.913	3.450	1.00	0.00	PROT
ATOM	1771	CD	GLJ	94	-13.506	9.070	5.505	1.00	0.00	PROT	1838	C	LVS	97	-7.075	10.316	1.934	1.00	0.00	PROT
ATOM	1772	OE1	GLJ	94	-13.835	8.052	6.091	1.00	0.00	PROT	1839	O	LVS	97	-6.083	10.862	2.376	1.00	0.00	PROT
ATOM	1773	OE2	GLJ	94	-12.429	9.624	5.652	1.00	0.00	PROT	1840	N	CYS	98	-7.235	9.024	2.029	1.00	0.00	PROT
ATOM	1774	C	GLJ	94	-12.114	8.639	2.083	1.00	0.00	PROT	1841	NN	CYS	98	-8.045	8.604	1.675	1.00	0.00	PROT
ATOM	1775	O	GLJ	94	-11.068	8.579	2.697	1.00	0.00	PROT	1842	CA	CYS	98	-6.196	8.169	2.699	1.00	0.00	PROT
ATOM	1776	N	TYR	95	-12.387	7.795	1.131	1.00	0.00	PROT	1843	HA	CYS	98	-5.857	8.169	2.699	1.00	0.00	PROT
ATOM	1777	NN	TYR	95	-13.236	7.862	0.646	1.00	0.00	PROT	1844	CA	CYS	98	-6.210	6.209	3.518	1.00	0.00	PROT
ATOM	1778	CA	TYR	95	-11.394	6.747	0.768	1.00	0.00	PROT	1845	HB1	CYS	98	-6.210	6.209	3.518	1.00	0.00	PROT
ATOM	1779	HA	TYR	95	-11.000	6.278	1.657	1.00	0.00	PROT	1846	HB2	CYS	98	-7.244	6.419	2.109	1.00	0.00	PROT
ATOM	1780	CB	TYR	95	-12.180	5.731	-0.064	1.00	0.00	PROT	1847	HG	CYS	98	-8.314	7.196	4.110	1.00	0.00	PROT
ATOM	1781	HB1	TYR	95	-11.681	5.577	-1.010	1.00	0.00	PROT	1848	HG	CYS	98	-9.117	7.036	3.608	1.00	0.00	PROT
ATOM	1782	HB2	TYR	95	-13.178	6.104	-0.239	1.00	0.00	PROT	1849	C	CYS	98	-5.018	7.927	1.762	1.00	0.00	PROT
ATOM	1783	CD	TYR	95	-12.255	4.421	0.683	1.00	0.00	PROT	1850	O	CYS	98	-3.923	8.407	1.980	1.00	0.00	PROT
ATOM	1784	CD1	TYR	95	-13.277	4.205	1.617	1.00	0.00	PROT	1851	N	ALA	99	-5.225	7.160	0.721	1.00	0.00	PROT
ATOM	1785	HD1	TYR	95	-14.011	4.975	1.845	1.00	0.00	PROT	1852	NN	ALA	99	-6.115	6.776	0.561	1.00	0.00	PROT
ATOM	1786	CD2	TYR	95	-11.503	3.422	0.401	1.00	0.00	PROT	1853	CA	ALA	99	-4.104	6.863	-0.219	1.00	0.00	PROT
ATOM	1787	HD2	TYR	95	-10.516	3.589	-0.273	1.00	0.00	PROT	1854	HA	ALA	99	-3.401	6.186	0.243	1.00	0.00	PROT
ATOM	1788	CE1	TYR	95	-13.346	2.991	-2.310	1.00	0.00	PROT	1855	HA	ALA	99	-4.764	6.193	-1.425	1.00	0.00	PROT
ATOM	1789	HE1	TYR	95	-14.134	2.824	3.030	1.00	0.00	PROT	1856	CE1	ALA	99	-5.133	6.951	-2.100	1.00	0.00	PROT

END

Table 11: Chemical Shifts

```

vector do (rmsd = 4.611 ) (resid 202 and name HA )
vector do (rmsd = 3.117 ) (resid 202 and name HB1 )
vector do (rmsd = 2.895 ) (resid 202 and name HB2 )
vector do (rmsd = 7.126 ) (resid 202 and name HD1 )
vector do (rmsd = 7.126 ) (resid 202 and name HD2 )
vector do (rmsd = 6.846 ) (resid 202 and name HE1 )
vector do (rmsd = 6.846 ) (resid 202 and name HE2 )
vector do (rmsd = 3.921 ) (resid 203 and name HA1 )
vector do (rmsd = 3.921 ) (resid 203 and name HA2 )
vector do (rmsd = 4.418 ) (resid 204 and name HA )
vector do (rmsd = 1.862 ) (resid 204 and name HB1 )
vector do (rmsd = 1.775 ) (resid 204 and name HB2 )
vector do (rmsd = 1.644 ) (resid 204 and name HG1 )
vector do (rmsd = 3.190 ) (resid 204 and name HD1 )
vector do (rmsd = 4.289 ) (resid 205 and name HA )
vector do (rmsd = 1.765 ) (resid 205 and name HB1 )
vector do (rmsd = 1.295 ) (resid 205 and name HG1 )
vector do (rmsd = 1.145 ) (resid 205 and name HG2 )
vector do (rmsd = 1.415 ) (resid 205 and name HD1 )
vector do (rmsd = 3.072 ) (resid 205 and name HE1 )
vector do (rmsd = 7.881 ) (resid 205 and name HZ )
vector do (rmsd = 1.872 ) (resid 205 and name HH# )
vector do (rmsd = 4.312 ) (resid 206 and name HA )
vector do (rmsd = 1.440 ) (resid 206 and name HG1 )
vector do (rmsd = 3.156 ) (resid 206 and name HE1 )
vector do (rmsd = 4.296 ) (resid 207 and name HA )
vector do (rmsd = 1.805 ) (resid 207 and name HB1 )
vector do (rmsd = 1.660 ) (resid 207 and name HG1 )
vector do (rmsd = 3.202 ) (resid 207 and name HD1 )
vector do (rmsd = 4.310 ) (resid 208 and name HA )
vector do (rmsd = 1.776 ) (resid 208 and name HB1 )
vector do (rmsd = 1.613 ) (resid 208 and name HG1 )
vector do (rmsd = 3.149 ) (resid 208 and name HD1 )
vector do (rmsd = 4.314 ) (resid 209 and name HA )
vector do (rmsd = 2.073 ) (resid 209 and name HB1 )
vector do (rmsd = 1.977 ) (resid 209 and name HB2 )
vector do (rmsd = 2.356 ) (resid 209 and name HG1 )
vector do (rmsd = 7.328 ) (resid 209 and name HE21)
vector do (rmsd = 6.862 ) (resid 209 and name HE22)
vector do (rmsd = 4.315 ) (resid 210 and name HA )
vector do (rmsd = 1.795 ) (resid 210 and name HB1 )
vector do (rmsd = 1.626 ) (resid 210 and name HG1 )
vector do (rmsd = 3.149 ) (resid 210 and name HD1 )
vector do (rmsd = 4.465 ) (resid 211 and name HA )
vector do (rmsd = 2.910 ) (resid 211 and name HB1 )
vector do (rmsd = 58.274 ) (resid 5 and name CA )
vector do (rmsd = 4.465 ) (resid 5 and name HA )
vector do (rmsd = 63.709 ) (resid 5 and name CB )
vector do (rmsd = 3.905 ) (resid 5 and name HB2 )
vector do (rmsd = 56.036 ) (resid 6 and name CA )
vector do (rmsd = 4.375 ) (resid 6 and name HA )
vector do (rmsd = 32.965 ) (resid 6 and name CB )
vector do (rmsd = 1.885 ) (resid 6 and name HB1 )
vector do (rmsd = 1.790 ) (resid 6 and name HB2 )
vector do (rmsd = 24.718 ) (resid 6 and name CG )
vector do (rmsd = 1.447 ) (resid 6 and name HG1 )
vector do (rmsd = 1.432 ) (resid 6 and name HG2 )
vector do (rmsd = 28.968 ) (resid 6 and name CD )
vector do (rmsd = 1.680 ) (resid 6 and name HD1 )
vector do (rmsd = 41.812 ) (resid 6 and name CE )
vector do (rmsd = 3.008 ) (resid 6 and name HE1 )
vector do (rmsd = 54.337 ) (resid 7 and name CA )
vector do (rmsd = 4.584 ) (resid 7 and name HA )
vector do (rmsd = 29.653 ) (resid 7 and name CB )
vector do (rmsd = 2.078 ) (resid 7 and name HB1 )
vector do (rmsd = 1.943 ) (resid 7 and name HB2 )
vector do (rmsd = 35.919 ) (resid 7 and name CG )
vector do (rmsd = 2.302 ) (resid 7 and name HG1 )
vector do (rmsd = 63.005 ) (resid 8 and name CA )
vector do (rmsd = 4.457 ) (resid 8 and name HA )
vector do (rmsd = 31.877 ) (resid 8 and name CB )
vector do (rmsd = 2.299 ) (resid 8 and name HB1 )
vector do (rmsd = 1.913 ) (resid 8 and name HB2 )
vector do (rmsd = 27.421 ) (resid 8 and name CG )
vector do (rmsd = 2.058 ) (resid 8 and name HG1 )
vector do (rmsd = 50.560 ) (resid 8 and name CD )
vector do (rmsd = 3.724 ) (resid 8 and name HD2 )
vector do (rmsd = 3.869 ) (resid 8 and name HD1 )
vector do (rmsd = 55.787 ) (resid 9 and name CA )
vector do (rmsd = 4.357 ) (resid 9 and name HA )
vector do (rmsd = 30.898 ) (resid 9 and name CB )
vector do (rmsd = 1.873 ) (resid 9 and name HB1 )
vector do (rmsd = 1.831 ) (resid 9 and name HB2 )
vector do (rmsd = 27.211 ) (resid 9 and name CG )
vector do (rmsd = 1.689 ) (resid 9 and name HG1 )

```

```

vector do (rmsd = 43.342 ) (resid 9 and name CD )
vector do (rmsd = 3.221 ) (resid 9 and name HD1 )
vector do (rmsd = 52.302 ) (resid 10 and name CA )
vector do (rmsd = 4.913 ) (resid 10 and name HA )
vector do (rmsd = 41.450 ) (resid 10 and name CB )
vector do (rmsd = 2.800 ) (resid 10 and name HB1 )
vector do (rmsd = 2.734 ) (resid 10 and name HB2 )
vector do (rmsd = 64.747 ) (resid 11 and name CA )
vector do (rmsd = 4.375 ) (resid 11 and name HA )
vector do (rmsd = 32.391 ) (resid 11 and name CB )
vector do (rmsd = 2.356 ) (resid 11 and name HB1 )
vector do (rmsd = 2.086 ) (resid 11 and name HB2 )
vector do (rmsd = 27.470 ) (resid 11 and name CG )
vector do (rmsd = 2.098 ) (resid 11 and name HG1 )
vector do (rmsd = 50.809 ) (resid 11 and name CD )
vector do (rmsd = 3.907 ) (resid 11 and name HD1 )
vector do (rmsd = 55.837 ) (resid 12 and name CA )
vector do (rmsd = 4.717 ) (resid 12 and name HA )
vector do (rmsd = 40.853 ) (resid 12 and name CB )
vector do (rmsd = 2.848 ) (resid 12 and name HB1 )
vector do (rmsd = 2.794 ) (resid 12 and name HB2 )
vector do (rmsd = 58.276 ) (resid 13 and name CA )
vector do (rmsd = 4.217 ) (resid 13 and name HA )
vector do (rmsd = 28.906 ) (resid 13 and name CB )
vector do (rmsd = 2.188 ) (resid 13 and name HB1 )
vector do (rmsd = 33.852 ) (resid 13 and name CG )
vector do (rmsd = 2.530 ) (resid 13 and name HG1 )
vector do (rmsd = 2.421 ) (resid 13 and name HG2 )
vector do (rmsd = 58.276 ) (resid 14 and name CA )
vector do (rmsd = 4.098 ) (resid 14 and name HA )
vector do (rmsd = 41.102 ) (resid 14 and name CB )
vector do (rmsd = 1.874 ) (resid 14 and name HB1 )
vector do (rmsd = 1.595 ) (resid 14 and name HB2 )
vector do (rmsd = 26.915 ) (resid 14 and name CG )
vector do (rmsd = 1.424 ) (resid 14 and name HG )
vector do (rmsd = 25.671 ) (resid 14 and name CD1 )
vector do (rmsd = 0.855 ) (resid 14 and name HD1# )
vector do (rmsd = 23.182 ) (resid 14 and name CD2 )
vector do (rmsd = 0.833 ) (resid 14 and name HD2# )
vector do (rmsd = 62.071 ) (resid 15 and name CA )
vector do (rmsd = 4.055 ) (resid 15 and name HA )
vector do (rmsd = 38.561 ) (resid 15 and name CB )
vector do (rmsd = 3.346 ) (resid 15 and name HB1 )
vector do (rmsd = 3.084 ) (resid 15 and name HB2 )
vector do (rmsd = 132.705 ) (resid 15 and name CD1 )
vector do (rmsd = 7.126 ) (resid 15 and name HD1 )
vector do (rmsd = 118.507 ) (resid 15 and name CE1 )
vector do (rmsd = 6.925 ) (resid 15 and name HE1 )
vector do (rmsd = 57.529 ) (resid 16 and name CA )
vector do (rmsd = 4.188 ) (resid 16 and name HA )
vector do (rmsd = 62.009 ) (resid 16 and name CB )
vector do (rmsd = 4.023 ) (resid 16 and name HB1 )
vector do (rmsd = 3.940 ) (resid 16 and name HB2 )
vector do (rmsd = 66.738 ) (resid 17 and name CA )
vector do (rmsd = 3.975 ) (resid 17 and name HA )
vector do (rmsd = 68.481 ) (resid 17 and name CB )
vector do (rmsd = 4.267 ) (resid 17 and name HB )
vector do (rmsd = 21.440 ) (resid 17 and name CG2 )
vector do (rmsd = 1.177 ) (resid 17 and name HG2# )
vector do (rmsd = 57.778 ) (resid 18 and name CA )
vector do (rmsd = 3.303 ) (resid 18 and name HA )
vector do (rmsd = 39.609 ) (resid 18 and name CB )
vector do (rmsd = 1.556 ) (resid 18 and name HB1 )
vector do (rmsd = 0.346 ) (resid 18 and name HB2 )
vector do (rmsd = 24.675 ) (resid 18 and name CG )
vector do (rmsd = 1.698 ) (resid 18 and name HG )
vector do (rmsd = 25.422 ) (resid 18 and name CD1 )
vector do (rmsd = 0.514 ) (resid 18 and name HD1# )
vector do (rmsd = 19.983 ) (resid 18 and name CD2 )
vector do (rmsd = -0.159 ) (resid 18 and name HD2# )
vector do (rmsd = 59.898 ) (resid 19 and name CA )
vector do (rmsd = 3.720 ) (resid 19 and name HA )
vector do (rmsd = 32.391 ) (resid 19 and name CB )
vector do (rmsd = 1.737 ) (resid 19 and name HB1 )
vector do (rmsd = 1.410 ) (resid 19 and name HB2 )
vector do (rmsd = 24.702 ) (resid 19 and name CG )
vector do (rmsd = 1.307 ) (resid 19 and name HG1 )
vector do (rmsd = 29.721 ) (resid 19 and name CD )
vector do (rmsd = 1.647 ) (resid 19 and name HD1 )
vector do (rmsd = 41.600 ) (resid 19 and name CE )
vector do (rmsd = 2.967 ) (resid 19 and name HE1 )
vector do (rmsd = 61.263 ) (resid 20 and name CA )
vector do (rmsd = 4.324 ) (resid 20 and name HA )
vector do (rmsd = 62.759 ) (resid 20 and name CB )
vector do (rmsd = 4.099 ) (resid 20 and name HB1 )
vector do (rmsd = 65.245 ) (resid 21 and name CA )
vector do (rmsd = 3.798 ) (resid 21 and name HA )

```

```

vector do (rmsd = 37.547 ) (resid 21 and name CB )
vector do (rmsd = 1.953 ) (resid 21 and name HB )
vector do (rmsd = 28.409 ) (resid 21 and name CG1 )
vector do (rmsd = 1.781 ) (resid 21 and name HG11 )
vector do (rmsd = 1.077 ) (resid 21 and name HG12 )
vector do (rmsd = 17.208 ) (resid 21 and name CG2 )
vector do (rmsd = 1.016 ) (resid 21 and name HG2# )
vector do (rmsd = 13.433 ) (resid 21 and name CD1 )
vector do (rmsd = 0.651 ) (resid 21 and name HD1# )
vector do (rmsd = 58.276 ) (resid 22 and name CA )
vector do (rmsd = 4.147 ) (resid 22 and name HA )
vector do (rmsd = 41.600 ) (resid 22 and name CB )
vector do (rmsd = 2.126 ) (resid 22 and name HB1 )
vector do (rmsd = 1.736 ) (resid 22 and name HB2 )
vector do (rmsd = 27.413 ) (resid 22 and name CG )
vector do (rmsd = 1.799 ) (resid 22 and name HG )
vector do (rmsd = 26.418 ) (resid 22 and name CD1 )
vector do (rmsd = 1.106 ) (resid 22 and name HD1# )
vector do (rmsd = 23.776 ) (resid 22 and name CD2 )
vector do (rmsd = 1.049 ) (resid 22 and name HD2# )
vector do (rmsd = 59.520 ) (resid 23 and name CA )
vector do (rmsd = 4.078 ) (resid 23 and name HA )
vector do (rmsd = 28.160 ) (resid 23 and name CB )
vector do (rmsd = 2.359 ) (resid 23 and name HB1 )
vector do (rmsd = 2.247 ) (resid 23 and name HB2 )
vector do (rmsd = 33.884 ) (resid 23 and name CG )
vector do (rmsd = 2.591 ) (resid 23 and name HG1 )
vector do (rmsd = 2.484 ) (resid 23 and name HG2 )
vector do (rmsd = 59.520 ) (resid 24 and name CA )
vector do (rmsd = 4.227 ) (resid 24 and name HA )
vector do (rmsd = 29.653 ) (resid 24 and name CB )
vector do (rmsd = 2.519 ) (resid 24 and name HB1 )
vector do (rmsd = 2.418 ) (resid 24 and name HB2 )
vector do (rmsd = 35.353 ) (resid 24 and name CG )
vector do (rmsd = 2.890 ) (resid 24 and name HG1 )
vector do (rmsd = 2.502 ) (resid 24 and name HG2 )
vector do (rmsd = 180.060 ) (resid 24 and name CD )
vector do (rmsd = 67.236 ) (resid 25 and name CA )
vector do (rmsd = 3.864 ) (resid 25 and name HA )
vector do (rmsd = 31.644 ) (resid 25 and name CB )
vector do (rmsd = 2.437 ) (resid 25 and name HB )
vector do (rmsd = 22.933 ) (resid 25 and name CG1 )
vector do (rmsd = 1.244 ) (resid 25 and name HG1# )
vector do (rmsd = 22.186 ) (resid 25 and name CG2 )
vector do (rmsd = 1.076 ) (resid 25 and name HG2# )
vector do (rmsd = 59.520 ) (resid 26 and name CA )
vector do (rmsd = 3.926 ) (resid 26 and name HA )
vector do (rmsd = 32.640 ) (resid 26 and name CB )
vector do (rmsd = 1.896 ) (resid 26 and name HB1 )
vector do (rmsd = 26.666 ) (resid 26 and name CG )
vector do (rmsd = 1.532 ) (resid 26 and name HG1 )
vector do (rmsd = 31.147 ) (resid 26 and name CD )
vector do (rmsd = 1.839 ) (resid 26 and name HD1 )
vector do (rmsd = 41.102 ) (resid 26 and name CE )
vector do (rmsd = 2.820 ) (resid 26 and name HE1 )
vector do (rmsd = 58.713 ) (resid 27 and name CA )
vector do (rmsd = 4.486 ) (resid 27 and name HA )
vector do (rmsd = 63.955 ) (resid 27 and name CB )
vector do (rmsd = 4.051 ) (resid 27 and name HB1 )
vector do (rmsd = 58.276 ) (resid 28 and name CA )
vector do (rmsd = 4.019 ) (resid 28 and name HA )
vector do (rmsd = 32.251 ) (resid 28 and name CB )
vector do (rmsd = 3.023 ) (resid 28 and name HB1 )
vector do (rmsd = 2.821 ) (resid 28 and name HB2 )
vector do (rmsd = 5.024 ) (resid 28 and name HD2 )
vector do (rmsd = 59.023 ) (resid 29 and name CA )
vector do (rmsd = 4.225 ) (resid 29 and name HA )
vector do (rmsd = 28.160 ) (resid 29 and name CB )
vector do (rmsd = 2.139 ) (resid 29 and name HB1 )
vector do (rmsd = 33.635 ) (resid 29 and name CG )
vector do (rmsd = 2.492 ) (resid 29 and name HG1 )
vector do (rmsd = 2.428 ) (resid 29 and name HG2 )
vector do (rmsd = 60.018 ) (resid 30 and name CA )
vector do (rmsd = 4.846 ) (resid 30 and name HA )
vector do (rmsd = 63.503 ) (resid 30 and name CB )
vector do (rmsd = 4.350 ) (resid 30 and name HB1 )
vector do (rmsd = 3.980 ) (resid 30 and name HB2 )
vector do (rmsd = 53.233 ) (resid 31 and name CA )
vector do (rmsd = 4.440 ) (resid 31 and name HA )
vector do (rmsd = 20.014 ) (resid 31 and name CB )
vector do (rmsd = 1.762 ) (resid 31 and name HB# )
vector do (rmsd = 60.570 ) (resid 32 and name CA )
vector do (rmsd = 4.423 ) (resid 32 and name HA )
vector do (rmsd = 27.911 ) (resid 32 and name CB )
vector do (rmsd = 3.637 ) (resid 32 and name HB1 )
vector do (rmsd = 3.408 ) (resid 32 and name HB2 )
vector do (rmsd = 127.381 ) (resid 32 and name CD1 )

```

```

vector do (rmsd = 7.889 ) (resid 32 and name HD1 )
vector do (rmsd = 10.403 ) (resid 32 and name HB1 )
vector do (rmsd = 7.359 ) (resid 32 and name HE3 )
vector do (rmsd = 7.190 ) (resid 32 and name HH2 )
vector do (rmsd = 64.498 ) (resid 33 and name CA )
vector do (rmsd = 3.990 ) (resid 33 and name HA )
vector do (rmsd = 30.151 ) (resid 33 and name CB )
vector do (rmsd = 1.078 ) (resid 33 and name HB1 )
vector do (rmsd = -0.432 ) (resid 33 and name HB2 )
vector do (rmsd = 25.671 ) (resid 33 and name CG )
vector do (rmsd = 0.271 ) (resid 33 and name HG1 )
vector do (rmsd = -0.875 ) (resid 33 and name HG2 )
vector do (rmsd = 50.062 ) (resid 33 and name CD )
vector do (rmsd = 1.570 ) (resid 33 and name HD2 )
vector do (rmsd = 2.268 ) (resid 33 and name HD1 )
vector do (rmsd = 55.777 ) (resid 34 and name CA )
vector do (rmsd = 5.005 ) (resid 34 and name HA )
vector do (rmsd = 39.111 ) (resid 34 and name CB )
vector do (rmsd = 3.516 ) (resid 34 and name HB1 )
vector do (rmsd = 2.613 ) (resid 34 and name HB2 )
vector do (rmsd = 7.180 ) (resid 34 and name HD1 )
vector do (rmsd = 7.199 ) (resid 34 and name HE1 )
vector do (rmsd = 7.278 ) (resid 34 and name HZ )
vector do (rmsd = 57.031 ) (resid 35 and name CA )
vector do (rmsd = 4.325 ) (resid 35 and name HA )
vector do (rmsd = 32.391 ) (resid 35 and name CB )
vector do (rmsd = 2.314 ) (resid 35 and name HB1 )
vector do (rmsd = 2.224 ) (resid 35 and name HB2 )
vector do (rmsd = 33.138 ) (resid 35 and name CG )
vector do (rmsd = 2.902 ) (resid 35 and name HG1 )
vector do (rmsd = 16.753 ) (resid 35 and name CE )
vector do (rmsd = 2.217 ) (resid 35 and name HE# )
vector do (rmsd = 53.298 ) (resid 36 and name CA )
vector do (rmsd = 4.867 ) (resid 36 and name HA )
vector do (rmsd = 31.395 ) (resid 36 and name CB )
vector do (rmsd = 2.149 ) (resid 36 and name HB1 )
vector do (rmsd = 1.800 ) (resid 36 and name HB2 )
vector do (rmsd = 35.905 ) (resid 36 and name CG )
vector do (rmsd = 2.205 ) (resid 36 and name HG1 )
vector do (rmsd = 63.005 ) (resid 37 and name CA )
vector do (rmsd = 4.271 ) (resid 37 and name HA )
vector do (rmsd = 31.921 ) (resid 37 and name CB )
vector do (rmsd = 2.381 ) (resid 37 and name HB1 )
vector do (rmsd = 1.703 ) (resid 37 and name HB2 )
vector do (rmsd = 27.164 ) (resid 37 and name CG )
vector do (rmsd = 2.182 ) (resid 37 and name HG1 )
vector do (rmsd = 2.040 ) (resid 37 and name HG2 )
vector do (rmsd = 50.560 ) (resid 37 and name CD )
vector do (rmsd = 3.706 ) (resid 37 and name HD1 )
vector do (rmsd = 63.752 ) (resid 38 and name CA )
vector do (rmsd = 3.492 ) (resid 38 and name HA )
vector do (rmsd = 32.139 ) (resid 38 and name CB )
vector do (rmsd = 1.071 ) (resid 38 and name HB )
vector do (rmsd = 22.188 ) (resid 38 and name CG1 )
vector do (rmsd = 0.498 ) (resid 38 and name HG1# )
vector do (rmsd = 21.440 ) (resid 38 and name CG2 )
vector do (rmsd = -0.008 ) (resid 38 and name HG2# )
vector do (rmsd = 56.815 ) (resid 39 and name CA )
vector do (rmsd = 4.441 ) (resid 39 and name HA )
vector do (rmsd = 32.142 ) (resid 39 and name CB )
vector do (rmsd = 2.033 ) (resid 39 and name HB1 )
vector do (rmsd = 1.924 ) (resid 39 and name HB2 )
vector do (rmsd = 25.671 ) (resid 39 and name CG )
vector do (rmsd = 1.644 ) (resid 39 and name HG1 )
vector do (rmsd = 1.463 ) (resid 39 and name HG2 )
vector do (rmsd = 28.906 ) (resid 39 and name CD )
vector do (rmsd = 1.715 ) (resid 39 and name HD1 )
vector do (rmsd = 1.644 ) (resid 39 and name HD2 )
vector do (rmsd = 40.356 ) (resid 39 and name CE )
vector do (rmsd = 3.186 ) (resid 39 and name HE1 )
vector do (rmsd = 2.950 ) (resid 39 and name HE2 )
vector do (rmsd = 3.679 ) (resid 40 and name HA )
vector do (rmsd = 62.756 ) (resid 41 and name CA )
vector do (rmsd = 4.097 ) (resid 41 and name HA )
vector do (rmsd = 68.441 ) (resid 41 and name CB )
vector do (rmsd = 4.343 ) (resid 41 and name HB )
vector do (rmsd = 22.435 ) (resid 41 and name CG2 )
vector do (rmsd = 1.320 ) (resid 41 and name HG2# )
vector do (rmsd = 56.145 ) (resid 42 and name CA )
vector do (rmsd = 4.501 ) (resid 42 and name HA )
vector do (rmsd = 30.874 ) (resid 42 and name CB )
vector do (rmsd = 2.217 ) (resid 42 and name HB1 )
vector do (rmsd = 2.075 ) (resid 42 and name HB2 )
vector do (rmsd = 36.637 ) (resid 42 and name CG )
vector do (rmsd = 2.362 ) (resid 42 and name HG1 )
vector do (rmsd = 2.268 ) (resid 42 and name HG2 )
vector do (rmsd = 49.565 ) (resid 43 and name CA )

```


vector do (rmsd = 5.000) (resid 43 and name HA)
vector do (rmsd = 20.427) (resid 43 and name CB)
vector do (rmsd = 0.969) (resid 43 and name HB#)
vector do (rmsd = 64.249) (resid 44 and name CA)
vector do (rmsd = 4.549) (resid 44 and name HA)
vector do (rmsd = 31.644) (resid 44 and name CB)
vector do (rmsd = 2.415) (resid 44 and name HB1)
vector do (rmsd = 2.053) (resid 44 and name HB2)
vector do (rmsd = 27.662) (resid 44 and name CG)
vector do (rmsd = 2.209) (resid 44 and name HG1)
vector do (rmsd = 2.079) (resid 44 and name HG2)
vector do (rmsd = 50.311) (resid 44 and name CD)
vector do (rmsd = 3.564) (resid 44 and name HD2)
vector do (rmsd = 3.838) (resid 44 and name HD1)
vector do (rmsd = 43.342) (resid 45 and name CA)
vector do (rmsd = 3.912) (resid 45 and name HA1)
vector do (rmsd = 62.697) (resid 46 and name CA)
vector do (rmsd = 3.506) (resid 46 and name HA)
vector do (rmsd = 39.609) (resid 46 and name CB)
vector do (rmsd = 2.784) (resid 46 and name HB1)
vector do (rmsd = 2.400) (resid 46 and name HB2)
vector do (rmsd = 5.998) (resid 46 and name HE1)
vector do (rmsd = 60.516) (resid 47 and name CA)
vector do (rmsd = 4.148) (resid 47 and name HA)
vector do (rmsd = 36.871) (resid 47 and name CB)
vector do (rmsd = 3.236) (resid 47 and name HB1)
vector do (rmsd = 2.861) (resid 47 and name HB2)
vector do (rmsd = 133.149) (resid 47 and name CD1)
vector do (rmsd = 7.409) (resid 47 and name HD1)
vector do (rmsd = 117.620) (resid 47 and name CE1)
vector do (rmsd = 6.675) (resid 47 and name HE1)
vector do (rmsd = 57.529) (resid 48 and name CA)
vector do (rmsd = 4.097) (resid 48 and name HA)
vector do (rmsd = 30.898) (resid 48 and name CB)
vector do (rmsd = 2.127) (resid 48 and name HB1)
vector do (rmsd = 2.104) (resid 48 and name HB2)
vector do (rmsd = 37.120) (resid 48 and name CG)
vector do (rmsd = 2.352) (resid 48 and name HG1)
vector do (rmsd = 2.247) (resid 48 and name HG2)
vector do (rmsd = 63.005) (resid 49 and name CA)
vector do (rmsd = 4.110) (resid 49 and name HA)
vector do (rmsd = 33.635) (resid 49 and name CB)
vector do (rmsd = 1.926) (resid 49 and name HB)
vector do (rmsd = 20.195) (resid 49 and name CG1)
vector do (rmsd = 0.990) (resid 49 and name HG1#)
vector do (rmsd = 20.957) (resid 49 and name CG2)
vector do (rmsd = 0.917) (resid 49 and name HG2#)
vector do (rmsd = 57.280) (resid 50 and name CA)
vector do (rmsd = 3.948) (resid 50 and name HA)
vector do (rmsd = 34.133) (resid 50 and name CB)
vector do (rmsd = 1.256) (resid 50 and name HB)
vector do (rmsd = 24.426) (resid 50 and name CG1)
vector do (rmsd = 0.826) (resid 50 and name HG11)
vector do (rmsd = 0.190) (resid 50 and name HG12)
vector do (rmsd = 16.175) (resid 50 and name CG2)
vector do (rmsd = 0.420) (resid 50 and name HG2#)
vector do (rmsd = 9.173) (resid 50 and name CD1)
vector do (rmsd = 0.582) (resid 50 and name HD1#)
vector do (rmsd = 57.031) (resid 51 and name CA)
vector do (rmsd = 3.876) (resid 51 and name HA)
vector do (rmsd = 30.400) (resid 51 and name CB)
vector do (rmsd = 1.396) (resid 51 and name HB1)
vector do (rmsd = 1.214) (resid 51 and name HB2)
vector do (rmsd = 26.915) (resid 51 and name CG)
vector do (rmsd = 1.350) (resid 51 and name HG1)
vector do (rmsd = 1.196) (resid 51 and name HG2)
vector do (rmsd = 42.638) (resid 51 and name CD)
vector do (rmsd = 3.025) (resid 51 and name HD1)
vector do (rmsd = 54.294) (resid 52 and name CA)
vector do (rmsd = 5.037) (resid 52 and name HA)
vector do (rmsd = 38.566) (resid 52 and name CB)
vector do (rmsd = 3.088) (resid 52 and name HB1)
vector do (rmsd = 2.955) (resid 52 and name HB2)
vector do (rmsd = 132.262) (resid 52 and name CD1)
vector do (rmsd = 7.281) (resid 52 and name HD1)
vector do (rmsd = 63.005) (resid 53 and name CA)
vector do (rmsd = 4.112) (resid 53 and name HA)
vector do (rmsd = 32.391) (resid 53 and name CB)
vector do (rmsd = 2.249) (resid 53 and name HB1)
vector do (rmsd = 27.911) (resid 53 and name CG)
vector do (rmsd = 2.275) (resid 53 and name HG1)
vector do (rmsd = 1.941) (resid 53 and name HG2)
vector do (rmsd = 50.311) (resid 53 and name CD)
vector do (rmsd = 3.446) (resid 53 and name HD2)
vector do (rmsd = 3.649) (resid 53 and name HD1)
vector do (rmsd = 53.547) (resid 54 and name CA)
vector do (rmsd = 4.987) (resid 54 and name HA)

vector do (rmsd = 31.147) (resid 54 and name CB)
vector do (rmsd = 2.057) (resid 54 and name HB1)
vector do (rmsd = 1.386) (resid 54 and name HB2)
vector do (rmsd = 30.649) (resid 54 and name CG)
vector do (rmsd = 2.737) (resid 54 and name HG1)
vector do (rmsd = 1.898) (resid 54 and name HG2)
vector do (rmsd = 14.027) (resid 54 and name CE)
vector do (rmsd = 2.002) (resid 54 and name HE#)
vector do (rmsd = 53.298) (resid 55 and name CA)
vector do (rmsd = 4.779) (resid 55 and name HA)
vector do (rmsd = 44.089) (resid 55 and name CB)
vector do (rmsd = 2.409) (resid 55 and name HB1)
vector do (rmsd = 57.529) (resid 56 and name CA)
vector do (rmsd = 4.075) (resid 56 and name HA)
vector do (rmsd = 41.102) (resid 56 and name CB)
vector do (rmsd = 2.115) (resid 56 and name HB1)
vector do (rmsd = 1.442) (resid 56 and name HB2)
vector do (rmsd = 27.150) (resid 56 and name CG)
vector do (rmsd = 1.768) (resid 56 and name HG)
vector do (rmsd = 26.930) (resid 56 and name CD1)
vector do (rmsd = 0.980) (resid 56 and name HD1#)
vector do (rmsd = 22.535) (resid 56 and name CD2)
vector do (rmsd = 0.678) (resid 56 and name HD2#)
vector do (rmsd = 60.267) (resid 57 and name CA)
vector do (rmsd = 3.910) (resid 57 and name HA)
vector do (rmsd = 30.400) (resid 57 and name CB)
vector do (rmsd = 1.144) (resid 57 and name HB1)
vector do (rmsd = 1.149) (resid 57 and name HB2)
vector do (rmsd = 24.924) (resid 57 and name CG)
vector do (rmsd = 1.531) (resid 57 and name HG1)
vector do (rmsd = 29.385) (resid 57 and name CD)
vector do (rmsd = 1.752) (resid 57 and name HD1)
vector do (rmsd = 0.919) (resid 57 and name HD2)
vector do (rmsd = 43.813) (resid 57 and name CE)
vector do (rmsd = 2.614) (resid 57 and name HB1)
vector do (rmsd = 2.109) (resid 57 and name HB2)
vector do (rmsd = 66.738) (resid 58 and name CA)
vector do (rmsd = 3.880) (resid 58 and name HA)
vector do (rmsd = 67.236) (resid 58 and name CB)
vector do (rmsd = 4.119) (resid 58 and name HB)
vector do (rmsd = 21.900) (resid 58 and name CG2)
vector do (rmsd = 1.090) (resid 58 and name HG2#)
vector do (rmsd = 60.784) (resid 59 and name CA)
vector do (rmsd = 4.357) (resid 59 and name HA)
vector do (rmsd = 33.038) (resid 59 and name CB)
vector do (rmsd = 2.145) (resid 59 and name HB1)
vector do (rmsd = 1.936) (resid 59 and name HB2)
vector do (rmsd = 32.889) (resid 59 and name CG)
vector do (rmsd = 2.651) (resid 59 and name HG1)
vector do (rmsd = 2.558) (resid 59 and name HG2)
vector do (rmsd = 16.164) (resid 59 and name CE)
vector do (rmsd = 1.310) (resid 59 and name HE#)
vector do (rmsd = 62.615) (resid 60 and name CA)
vector do (rmsd = 4.445) (resid 60 and name HA)
vector do (rmsd = 62.650) (resid 60 and name CB)
vector do (rmsd = 4.248) (resid 60 and name HB1)
vector do (rmsd = 4.065) (resid 60 and name HB2)
vector do (rmsd = 59.321) (resid 61 and name CA)
vector do (rmsd = 4.102) (resid 61 and name HA)
vector do (rmsd = 28.906) (resid 61 and name CB)
vector do (rmsd = 2.248) (resid 61 and name HB1)
vector do (rmsd = 2.112) (resid 61 and name HB2)
vector do (rmsd = 36.111) (resid 61 and name CG)
vector do (rmsd = 2.409) (resid 61 and name HG1)
vector do (rmsd = 2.277) (resid 61 and name HG2)
vector do (rmsd = 60.237) (resid 62 and name CA)
vector do (rmsd = 3.919) (resid 62 and name HA)
vector do (rmsd = 32.652) (resid 62 and name CB)
vector do (rmsd = 2.069) (resid 62 and name HB1)
vector do (rmsd = 1.077) (resid 62 and name HB2)
vector do (rmsd = 1.733) (resid 62 and name HG1)
vector do (rmsd = 0.839) (resid 62 and name HG2)
vector do (rmsd = 42.587) (resid 62 and name CD)
vector do (rmsd = 2.581) (resid 62 and name HD1)
vector do (rmsd = 58.247) (resid 63 and name CA)
vector do (rmsd = 4.717) (resid 63 and name HA)
vector do (rmsd = 42.098) (resid 63 and name CB)
vector do (rmsd = 2.354) (resid 63 and name HB1)
vector do (rmsd = 1.978) (resid 63 and name HB2)
vector do (rmsd = 27.164) (resid 63 and name CG)
vector do (rmsd = 1.849) (resid 63 and name HG)
vector do (rmsd = 26.915) (resid 63 and name CD1)
vector do (rmsd = 0.918) (resid 63 and name HD1#)
vector do (rmsd = 25.422) (resid 63 and name CD2)
vector do (rmsd = 1.082) (resid 63 and name HD2#)
vector do (rmsd = 59.093) (resid 64 and name CA)
vector do (rmsd = 4.376) (resid 64 and name HA)


```

vector do (rmsd = 2.487 ) (resid 86 and name HE1 )
vector do (rmsd = 2.465 ) (resid 86 and name HE2 )
vector do (rmsd = 57.951 ) (resid 87 and name CA )
vector do (rmsd = 4.327 ) (resid 87 and name HA )
vector do (rmsd = 30.151 ) (resid 87 and name CB )
vector do (rmsd = 2.230 ) (resid 87 and name HB1 )
vector do (rmsd = 2.075 ) (resid 87 and name HB2 )
vector do (rmsd = 36.390 ) (resid 87 and name CG )
vector do (rmsd = 2.440 ) (resid 87 and name HG1 )
vector do (rmsd = 2.238 ) (resid 87 and name HG2 )
vector do (rmsd = 61.263 ) (resid 88 and name CA )
vector do (rmsd = 4.320 ) (resid 88 and name HA )
vector do (rmsd = 40.895 ) (resid 88 and name CB )
vector do (rmsd = 2.958 ) (resid 88 and name HB1 )
vector do (rmsd = 2.915 ) (resid 88 and name HB2 )
vector do (rmsd = 133.149 ) (resid 88 and name CD1 )
vector do (rmsd = 6.968 ) (resid 88 and name HD1 )
vector do (rmsd = 6.968 ) (resid 88 and name HD2 )
vector do (rmsd = 118.064 ) (resid 88 and name CE1 )
vector do (rmsd = 6.672 ) (resid 88 and name HE1 )
vector do (rmsd = 51.817 ) (resid 89 and name CA )
vector do (rmsd = 5.091 ) (resid 89 and name HA )
vector do (rmsd = 40.604 ) (resid 89 and name CB )
vector do (rmsd = 3.100 ) (resid 89 and name HB1 )
vector do (rmsd = 2.903 ) (resid 89 and name HB2 )
vector do (rmsd = 61.263 ) (resid 90 and name CA )
vector do (rmsd = 4.659 ) (resid 90 and name HA )
vector do (rmsd = 31.147 ) (resid 90 and name CB )
vector do (rmsd = 2.349 ) (resid 90 and name HB1 )
vector do (rmsd = 2.175 ) (resid 90 and name HB2 )
vector do (rmsd = 50.191 ) (resid 90 and name CD )
vector do (rmsd = 3.945 ) (resid 90 and name HD2 )
vector do (rmsd = 4.116 ) (resid 90 and name HD1 )
vector do (rmsd = 63.752 ) (resid 91 and name CA )
vector do (rmsd = 2.586 ) (resid 91 and name HA )
vector do (rmsd = 31.644 ) (resid 91 and name CB )
vector do (rmsd = 1.625 ) (resid 91 and name HB1 )
vector do (rmsd = 27.413 ) (resid 91 and name CG )
vector do (rmsd = 1.994 ) (resid 91 and name HG1 )
vector do (rmsd = 1.708 ) (resid 91 and name HG2 )
vector do (rmsd = 57.018 ) (resid 92 and name CA )
vector do (rmsd = 4.252 ) (resid 92 and name HA )
vector do (rmsd = 28.160 ) (resid 92 and name CB )
vector do (rmsd = 2.105 ) (resid 92 and name HB1 )
vector do (rmsd = 2.023 ) (resid 92 and name HB2 )
vector do (rmsd = 37.120 ) (resid 92 and name CG )
vector do (rmsd = 2.387 ) (resid 92 and name HG1 )
vector do (rmsd = 2.263 ) (resid 92 and name HG2 )
vector do (rmsd = 64.000 ) (resid 93 and name CA )
vector do (rmsd = 4.527 ) (resid 93 and name HA )
vector do (rmsd = 67.236 ) (resid 93 and name CB )
vector do (rmsd = 3.873 ) (resid 93 and name HB1 )
vector do (rmsd = 59.082 ) (resid 94 and name CA )
vector do (rmsd = 4.244 ) (resid 94 and name HA )
vector do (rmsd = 28.658 ) (resid 94 and name CB )
vector do (rmsd = 2.144 ) (resid 94 and name HB1 )
vector do (rmsd = 2.035 ) (resid 94 and name HB2 )
vector do (rmsd = 36.079 ) (resid 94 and name CG )
vector do (rmsd = 2.257 ) (resid 94 and name HG1 )
vector do (rmsd = 61.125 ) (resid 95 and name CA )
vector do (rmsd = 3.651 ) (resid 95 and name HA )
vector do (rmsd = 38.613 ) (resid 95 and name CB )
vector do (rmsd = 2.953 ) (resid 95 and name HB1 )
vector do (rmsd = 2.634 ) (resid 95 and name HB2 )
vector do (rmsd = 6.869 ) (resid 95 and name HD1 )
vector do (rmsd = 6.862 ) (resid 95 and name HD2 )
vector do (rmsd = 61.597 ) (resid 96 and name CA )
vector do (rmsd = 3.828 ) (resid 96 and name HA )
vector do (rmsd = 40.107 ) (resid 96 and name CB )
vector do (rmsd = 3.429 ) (resid 96 and name HB1 )
vector do (rmsd = 2.580 ) (resid 96 and name HB2 )
vector do (rmsd = 134.924 ) (resid 96 and name CD1 )
vector do (rmsd = 7.122 ) (resid 96 and name HD1 )
vector do (rmsd = 118.064 ) (resid 96 and name CE1 )
vector do (rmsd = 7.054 ) (resid 96 and name HE1 )
vector do (rmsd = 60.266 ) (resid 97 and name CA )
vector do (rmsd = 4.236 ) (resid 97 and name HA )
vector do (rmsd = 32.241 ) (resid 97 and name CB )
vector do (rmsd = 2.112 ) (resid 97 and name HB1 )
vector do (rmsd = 25.714 ) (resid 97 and name CG )
vector do (rmsd = 1.827 ) (resid 97 and name HG1 )
vector do (rmsd = 1.617 ) (resid 97 and name HG2 )
vector do (rmsd = 29.653 ) (resid 97 and name CD )
vector do (rmsd = 1.840 ) (resid 97 and name HD1 )
vector do (rmsd = 41.801 ) (resid 97 and name CE )
vector do (rmsd = 3.009 ) (resid 97 and name HE1 )
vector do (rmsd = 64.996 ) (resid 98 and name CA )

```

```

vector do (rmsd = 4.220 ) (resid 98 and name HA )
vector do (rmsd = 26.655 ) (resid 98 and name CB )
vector do (rmsd = 3.402 ) (resid 98 and name HB1 )
vector do (rmsd = 3.078 ) (resid 98 and name HB2 )
vector do (rmsd = 55.289 ) (resid 99 and name CA )
vector do (rmsd = 3.909 ) (resid 99 and name HA )
vector do (rmsd = 18.323 ) (resid 99 and name CB )
vector do (rmsd = 1.660 ) (resid 99 and name HB# )
vector do (rmsd = 55.753 ) (resid 100 and name CA )
vector do (rmsd = 4.362 ) (resid 100 and name HA )
vector do (rmsd = 38.726 ) (resid 100 and name CB )
vector do (rmsd = 2.916 ) (resid 100 and name HB1 )
vector do (rmsd = 2.851 ) (resid 100 and name HB2 )
vector do (rmsd = 64.747 ) (resid 101 and name CA )
vector do (rmsd = 3.693 ) (resid 101 and name HA )
vector do (rmsd = 38.862 ) (resid 101 and name CB )
vector do (rmsd = 1.947 ) (resid 101 and name HB )
vector do (rmsd = 29.404 ) (resid 101 and name CG1 )
vector do (rmsd = 1.885 ) (resid 101 and name HG11 )
vector do (rmsd = 1.241 ) (resid 101 and name HG12 )
vector do (rmsd = 17.706 ) (resid 101 and name CG2 )
vector do (rmsd = 1.032 ) (resid 101 and name HG2# )
vector do (rmsd = 13.475 ) (resid 101 and name CD1 )
vector do (rmsd = 0.993 ) (resid 101 and name HD1# )
vector do (rmsd = 56.534 ) (resid 102 and name CA )
vector do (rmsd = 3.722 ) (resid 102 and name HA )
vector do (rmsd = 41.600 ) (resid 102 and name CB )
vector do (rmsd = 1.484 ) (resid 102 and name HB1 )
vector do (rmsd = 1.266 ) (resid 102 and name HB2 )
vector do (rmsd = 26.666 ) (resid 102 and name CG )
vector do (rmsd = 1.591 ) (resid 102 and name HG )
vector do (rmsd = 25.173 ) (resid 102 and name CD1 )
vector do (rmsd = 0.763 ) (resid 102 and name HD1# )
vector do (rmsd = 24.190 ) (resid 102 and name CD2 )
vector do (rmsd = 0.766 ) (resid 102 and name HD2# )
vector do (rmsd = 59.520 ) (resid 103 and name CA )
vector do (rmsd = 3.222 ) (resid 103 and name HA )
vector do (rmsd = 29.816 ) (resid 103 and name CB )
vector do (rmsd = 1.801 ) (resid 103 and name HB1 )
vector do (rmsd = 1.333 ) (resid 103 and name HB2 )
vector do (rmsd = 37.065 ) (resid 103 and name CG )
vector do (rmsd = 2.043 ) (resid 103 and name HG1 )
vector do (rmsd = 1.957 ) (resid 103 and name HG2 )
vector do (rmsd = 59.520 ) (resid 104 and name CA )
vector do (rmsd = 4.112 ) (resid 104 and name HA )
vector do (rmsd = 32.185 ) (resid 104 and name CB )
vector do (rmsd = 1.960 ) (resid 104 and name HB1 )
vector do (rmsd = 25.246 ) (resid 104 and name CG )
vector do (rmsd = 1.557 ) (resid 104 and name HG1 )
vector do (rmsd = 1.464 ) (resid 104 and name HG2 )
vector do (rmsd = 29.053 ) (resid 104 and name CD )
vector do (rmsd = 1.706 ) (resid 104 and name HD1 )
vector do (rmsd = 41.855 ) (resid 104 and name CE )
vector do (rmsd = 3.036 ) (resid 104 and name HE1 )
vector do (rmsd = 61.431 ) (resid 105 and name CA )
vector do (rmsd = 4.352 ) (resid 105 and name HA )
vector do (rmsd = 39.111 ) (resid 105 and name CB )
vector do (rmsd = 3.138 ) (resid 105 and name HB1 )
vector do (rmsd = 3.101 ) (resid 105 and name HB2 )
vector do (rmsd = 131.818 ) (resid 105 and name CD1 )
vector do (rmsd = 7.242 ) (resid 105 and name HD1 )
vector do (rmsd = 60.516 ) (resid 106 and name CA )
vector do (rmsd = 3.997 ) (resid 106 and name HA )
vector do (rmsd = 38.592 ) (resid 106 and name CB )
vector do (rmsd = 3.356 ) (resid 106 and name HB1 )
vector do (rmsd = 3.134 ) (resid 106 and name HB2 )
vector do (rmsd = 132.262 ) (resid 106 and name CD1 )
vector do (rmsd = 6.956 ) (resid 106 and name HD1 )
vector do (rmsd = 61.512 ) (resid 107 and name CA )
vector do (rmsd = 3.857 ) (resid 107 and name HA )
vector do (rmsd = 37.867 ) (resid 107 and name CB )
vector do (rmsd = 3.098 ) (resid 107 and name HB1 )
vector do (rmsd = 131.374 ) (resid 107 and name CD1 )
vector do (rmsd = 7.239 ) (resid 107 and name HD1 )
vector do (rmsd = 61.512 ) (resid 108 and name CA )
vector do (rmsd = 4.236 ) (resid 108 and name HA )
vector do (rmsd = 62.591 ) (resid 108 and name CB )
vector do (rmsd = 4.022 ) (resid 108 and name HB1 )
vector do (rmsd = 56.783 ) (resid 109 and name CA )
vector do (rmsd = 4.074 ) (resid 109 and name HA )
vector do (rmsd = 31.644 ) (resid 109 and name CB )
vector do (rmsd = 1.770 ) (resid 109 and name HB1 )
vector do (rmsd = 1.587 ) (resid 109 and name HB2 )
vector do (rmsd = 23.020 ) (resid 109 and name CG )
vector do (rmsd = 0.852 ) (resid 109 and name HG1 )
vector do (rmsd = 27.005 ) (resid 109 and name CD )
vector do (rmsd = 1.417 ) (resid 109 and name HD1 )

```

```

vector do (rmsd = 42.098 ) (resid 109 and name CE )
vector do (rmsd = 2.618 ) (resid 109 and name HE1 )
vector do (rmsd = 2.483 ) (resid 109 and name HE2 )
vector do (rmsd = 64.249 ) (resid 110 and name CA )
vector do (rmsd = 3.854 ) (resid 110 and name HA )
vector do (rmsd = 37.120 ) (resid 110 and name CB )
vector do (rmsd = 1.796 ) (resid 110 and name HB )
vector do (rmsd = 26.418 ) (resid 110 and name CG1 )
vector do (rmsd = 1.162 ) (resid 110 and name HG11 )
vector do (rmsd = 1.090 ) (resid 110 and name HG12 )
vector do (rmsd = 18.619 ) (resid 110 and name CG2 )
vector do (rmsd = 0.693 ) (resid 110 and name HG2# )
vector do (rmsd = 13.226 ) (resid 110 and name CD1 )
vector do (rmsd = 0.571 ) (resid 110 and name HD1# )
vector do (rmsd = 59.520 ) (resid 111 and name CA )
vector do (rmsd = 4.094 ) (resid 111 and name HA )
vector do (rmsd = 32.858 ) (resid 111 and name CB )
vector do (rmsd = 1.930 ) (resid 111 and name HB1 )
vector do (rmsd = 1.793 ) (resid 111 and name HB2 )
vector do (rmsd = 25.195 ) (resid 111 and name CG )
vector do (rmsd = 1.453 ) (resid 111 and name HG1 )
vector do (rmsd = 1.350 ) (resid 111 and name HG2 )
vector do (rmsd = 29.409 ) (resid 111 and name CD )
vector do (rmsd = 1.664 ) (resid 111 and name HD1 )
vector do (rmsd = 41.351 ) (resid 111 and name CE )
vector do (rmsd = 2.942 ) (resid 111 and name HE1 )
vector do (rmsd = 58.525 ) (resid 112 and name CA )
vector do (rmsd = 4.025 ) (resid 112 and name HA )
vector do (rmsd = 30.077 ) (resid 112 and name CB )
vector do (rmsd = 2.097 ) (resid 112 and name HB1 )
vector do (rmsd = 36.227 ) (resid 112 and name CG )
vector do (rmsd = 2.394 ) (resid 112 and name HG1 )
vector do (rmsd = 2.252 ) (resid 112 and name HG2 )
vector do (rmsd = 52.302 ) (resid 113 and name CA )
vector do (rmsd = 4.354 ) (resid 113 and name HA )
vector do (rmsd = 19.449 ) (resid 113 and name CB )
vector do (rmsd = 1.405 ) (resid 113 and name HB# )
vector do (rmsd = 46.021 ) (resid 114 and name CA )
vector do (rmsd = 4.265 ) (resid 114 and name HA1 )
vector do (rmsd = 4.070 ) (resid 114 and name HA2 )
vector do (rmsd = 55.538 ) (resid 115 and name CA )
vector do (rmsd = 4.251 ) (resid 115 and name HA )
vector do (rmsd = 42.845 ) (resid 115 and name CB )
vector do (rmsd = 1.613 ) (resid 115 and name HB2 )
vector do (rmsd = 27.077 ) (resid 115 and name CG )
vector do (rmsd = 1.571 ) (resid 115 and name HG )
vector do (rmsd = 25.485 ) (resid 115 and name CD1 )
vector do (rmsd = 0.750 ) (resid 115 and name HD1# )
vector do (rmsd = 23.302 ) (resid 115 and name CD2 )
vector do (rmsd = 0.783 ) (resid 115 and name HD2# )
vector do (rmsd = 60.018 ) (resid 116 and name CA )
vector do (rmsd = 4.275 ) (resid 116 and name HA )
vector do (rmsd = 39.609 ) (resid 116 and name CB )
vector do (rmsd = 1.851 ) (resid 116 and name HB )
vector do (rmsd = 26.903 ) (resid 116 and name CG1 )
vector do (rmsd = 1.346 ) (resid 116 and name HG11 )
vector do (rmsd = 0.964 ) (resid 116 and name HG12 )
vector do (rmsd = 17.706 ) (resid 116 and name CG2 )
vector do (rmsd = 0.854 ) (resid 116 and name HG2# )
vector do (rmsd = 13.193 ) (resid 116 and name CD1 )
vector do (rmsd = 0.825 ) (resid 116 and name HD1# )
vector do (rmsd = 54.543 ) (resid 117 and name CA )
vector do (rmsd = 4.602 ) (resid 117 and name HA )
vector do (rmsd = 41.387 ) (resid 117 and name CB )
vector do (rmsd = 2.732 ) (resid 117 and name HB1 )
vector do (rmsd = 2.582 ) (resid 117 and name HB2 )
vector do (rmsd = 57.883 ) (resid 118 and name CA )
vector do (rmsd = 4.076 ) (resid 118 and name HA )
vector do (rmsd = 33.670 ) (resid 118 and name CB )
vector do (rmsd = 1.799 ) (resid 118 and name HB1 )
vector do (rmsd = 1.693 ) (resid 118 and name HB2 )
vector do (rmsd = 24.639 ) (resid 118 and name CG )
vector do (rmsd = 1.373 ) (resid 118 and name HG1 )
vector do (rmsd = 29.653 ) (resid 118 and name CD )
vector do (rmsd = 1.672 ) (resid 118 and name HD1 )
vector do (rmsd = 40.506 ) (resid 118 and name CE )
vector do (rmsd = 2.997 ) (resid 118 and name HE1 )

```

Table 12: Hydrogen Bond Distance Restraints

```

!Helix Z
assign (residue 19 and name HN ) (residue 15 and name O ) 1.80 0.0 0.40
assign (residue 19 and name N ) (residue 15 and name O ) 2.80 0.30 0.40

assign (residue 22 and name HN ) (residue 18 and name O ) 1.80 0.0 0.40
assign (residue 22 and name N ) (residue 18 and name O ) 2.80 0.30 0.40

assign (residue 23 and name HN ) (residue 19 and name O ) 1.80 0.0 0.40
assign (residue 23 and name N ) (residue 19 and name O ) 2.80 0.30 0.40

assign (residue 24 and name HN ) (residue 20 and name O ) 1.80 0.0 0.40
assign (residue 24 and name N ) (residue 20 and name O ) 2.80 0.30 0.40

assign (residue 25 and name HN ) (residue 21 and name O ) 1.80 0.0 0.40
assign (residue 25 and name N ) (residue 21 and name O ) 2.80 0.30 0.40

!Helix B
assign (residue 75 and name HN ) (residue 71 and name O ) 1.80 0.0 0.40
assign (residue 75 and name N ) (residue 71 and name O ) 2.80 0.30 0.40

!assign (residue 77 and name HN ) (residue 73 and name O ) 1.80 0.0 0.40
!assign (residue 77 and name N ) (residue 73 and name O ) 2.80 0.30 0.40

assign (residue 78 and name HN ) (residue 74 and name O ) 1.80 0.0 0.40
assign (residue 78 and name N ) (residue 74 and name O ) 2.80 0.30 0.40

assign (residue 79 and name HN ) (residue 75 and name O ) 1.80 0.0 0.40
assign (residue 79 and name N ) (residue 75 and name O ) 2.80 0.30 0.40

!assign (residue 80 and name HN ) (residue 76 and name O ) 1.80 0.0 0.40
!assign (residue 80 and name N ) (residue 76 and name O ) 2.80 0.30 0.40

assign (residue 81 and name HN ) (residue 77 and name O ) 1.80 0.0 0.40
assign (residue 81 and name N ) (residue 77 and name O ) 2.80 0.30 0.40

assign (residue 82 and name HN ) (residue 78 and name O ) 1.80 0.0 0.40
assign (residue 82 and name N ) (residue 78 and name O ) 2.80 0.30 0.40

!Helix C
assign (residue 102 and name HN ) (residue 98 and name O ) 1.80 0.0 0.40
assign (residue 102 and name N ) (residue 98 and name O ) 2.80 0.30 0.40

assign (residue 103 and name HN ) (residue 99 and name O ) 1.80 0.0 0.40
assign (residue 103 and name N ) (residue 99 and name O ) 2.80 0.30 0.40

assign (residue 104 and name HN ) (residue 100 and name O ) 1.80 0.0 0.40
assign (residue 104 and name N ) (residue 100 and name O ) 2.80 0.30 0.40

assign (residue 105 and name HN ) (residue 101 and name O ) 1.80 0.0 0.40
assign (residue 105 and name N ) (residue 101 and name O ) 2.80 0.30 0.40

```

Table 13 Unambiguous NOE Distance Restraints

ASSI { 1}	((segid "PROT" and resid 29 and name HN))								
	((segid "PROT" and resid 28 and name HN))								
	3.300 2.700 2.200 peak 1 weight	0.10000E+01 volume	0.18248E+01 ppm1	8.583 ppm2	7.565				
ASSI { 11}	((segid "PROT" and resid 29 and name HN))								
	((segid "PROT" and resid 29 and name HA))								
	2.700 1.800 1.800 peak 11 weight	0.10000E+01 volume	0.64796E+01 ppm1	8.584 ppm2	4.224				
ASSI { 21}	((segid "PROT" and resid 29 and name HN))								
	((segid "PROT" and resid 28 and name HA))								
	2.400 1.400 1.400 peak 21 weight	0.10000E+01 volume	0.14203E+02 ppm1	8.583 ppm2	3.997				
ASSI { 31}	((segid "PROT" and resid 29 and name HN))								
	((segid "PROT" and resid 28 and name HB1))								
	3.500 3.100 2.000 peak 31 weight	0.10000E+01 volume	0.14751E+01 ppm1	8.583 ppm2	3.019				
ASSI { 41}	((segid "PROT" and resid 29 and name HN))								
	((segid "PROT" and resid 29 and name HG2))								
	3.000 2.200 2.200 peak 41 weight	0.10000E+01 volume	0.37768E+01 ppm1	8.583 ppm2	2.419				
ASSI { 51}	((segid "PROT" and resid 29 and name HN))								
	((segid "PROT" and resid 29 and name HB1))								
	2.400 1.400 1.400 peak 51 weight	0.10000E+01 volume	0.13363E+02 ppm1	8.583 ppm2	2 125				
ASSI { 71}	((segid "PROT" and resid 29 and name HN))								
	((segid "PROT" and resid 28 and name HB2))								
	3.400 2.900 2.100 peak 71 weight	0.10000E+01 volume	0.15259E+01 ppm1	8.598 ppm2	2.776				
ASSI { 81}	((segid "PROT" and resid 57 and name HN))								
	((segid "PROT" and resid 57 and name HG1))								
	3.300 2.700 2.200 peak 81 weight	0.10000E+01 volume	0.19711E+01 ppm1	8.807 ppm2	1.511				
ASSI { 91}	((segid "PROT" and resid 57 and name HN))								
	((segid "PROT" and resid 58 and name HN))								
	2.600 1.700 1.700 peak 91 weight	0.10000E+01 volume	0.89521E+01 ppm1	8.801 ppm2	9.439				
ASSI { 101}	((segid "PROT" and resid 57 and name HN))								
	((segid "PROT" and resid 56 and name HN))								
	2.800 2.000 2.000 peak 101 weight	0.10000E+01 volume	0.49351E+01 ppm1	8.803 ppm2	9.125				
ASSI { 111}	((segid "PROT" and resid 57 and name HN))								
	((segid "PROT" and resid 59 and name HN))								
	3.400 2.900 2.100 peak 111 weight	0.10000E+01 volume	0.16857E+01 ppm1	8.801 ppm2	7.884				
ASSI { 121}	((segid "PROT" and resid 57 and name HN))								
	((segid "PROT" and resid 36 and name HA))								
	3.100 2.400 2.400 peak 121 weight	0.10000E+01 volume	0 30255E+01 ppm1	8.802 ppm2	4.847				
ASSI { 131}	((segid "PROT" and resid 57 and name HN))								
	((segid "PROT" and resid 55 and name HA))								
	2.900 2.100 2.100 peak 131 weight	0.10000E+01 volume	0.41647E+01 ppm1	8.802 ppm2	4.741				
ASSI { 151}	((segid "PROT" and resid 57 and name HN))								
	((segid "PROT" and resid 56 and name HA))								
	3.300 2.700 2.200 peak 151 weight	0.10000E+01 volume	0.19189E+01 ppm1	8.798 ppm2	4.063				
ASSI { 171}	((segid "PROT" and resid 57 and name HN))								
	((segid "PROT" and resid 55 and name HB1))								
	2.500 1.600 1.600 peak 171 weight	0.10000E+01 volume	0.95863E+01 ppm1	8.801 ppm2	2.371				
ASSI { 181}	((segid "PROT" and resid 57 and name HN))								
	((segid "PROT" and resid 35 and name HB1))								
	2.600 2.600 1.900 peak 181 weight	0.10000E+01 volume	0.84398E+01 ppm1	8.801 ppm2	2.269				
ASSI { 191}	((segid "PROT" and resid 57 and name HN))								
	((segid "PROT" and resid 56 and name HB1))								
	3.200 2.600 2.300 peak 191 weight	0.10000E+01 volume	0.24962E+01 ppm1	8.803 ppm2	2.090				
ASSI { 201}	((segid "PROT" and resid 57 and name HN))								
	((segid "PROT" and resid 57 and name HD1))								
	3.200 2.600 2.300 peak 201 weight	0.10000E+01 volume	0.24126E+01 ppm1	8.800 ppm2	1 724				
ASSI { 211}	((segid "PROT" and resid 57 and name HN))								
	((segid "PROT" and resid 56 and name HB2))								
	3.100 2.400 2.400 peak 211 weight	0.10000E+01 volume	0.27264E+01 ppm1	8.800 ppm2	1.424				
ASSI { 261}	((segid "PROT" and resid 118 and name HN))								
	((segid "PROT" and resid 117 and name HA))								
	2.200 1.200 1.200 peak 261 weight	0.10000E+01 volume	0.21965E+02 ppm1	7.777 ppm2	4.583				
ASSI { 271}	((segid "PROT" and resid 118 and name HN))								
	((segid "PROT" and resid 118 and name HA))								
	2.300 1.300 1 300 peak 271 weight	0.10000E+01 volume	0.15108E+02 ppm1	7.774 ppm2	4.076				
ASSI { 281}	((segid "PROT" and resid 118 and name HN))								

```

(( segid "PROT" and resid 117 and name HB1 ))
2.900 2.100 2.100 peak 281 weight 0.10000E+01 volume 0.45666E+01 ppm1 7.775 ppm2 2.710
ASSI { 291}
(( segid "PROT" and resid 118 and name HN ))
(( segid "PROT" and resid 117 and name HB2 ))
3.200 2.600 2.300 peak 291 weight 0.10000E+01 volume 0.21751E+01 ppm1 7.775 ppm2 2.569
ASSI { 301}
(( segid "PROT" and resid 118 and name HN ))
(( segid "PROT" and resid 118 and name HB1 ))
2.800 2.000 2.000 peak 301 weight 0.10000E+01 volume 0.47059E+01 ppm1 7.776 ppm2 1.799
ASSI { 311}
(( segid "PROT" and resid 118 and name HN ))
(( segid "PROT" and resid 118 and name HB2 ))
2.600 1.700 1.700 peak 311 weight 0.10000E+01 volume 0.80279E+01 ppm1 7.776 ppm2 1.693
ASSI { 321}
(( segid "PROT" and resid 118 and name HN ))
(( segid "PROT" and resid 116 and name HD1% ))
3.000 2.200 2.200 peak 321 weight 0.10000E+01 volume 0.36749E+01 ppm1 7.773 ppm2 0.824
ASSI { 331}
(( segid "PROT" and resid 118 and name HN ))
(( segid "PROT" and resid 116 and name HN ))
2.700 1.800 1.800 peak 331 weight 0.10000E+01 volume 0.67264E+01 ppm1 7.768 ppm2 7.476
ASSI { 341}
(( segid "PROT" and resid 51 and name HN ))
(( segid "PROT" and resid 49 and name HN ))
3.200 2.600 2.300 peak 341 weight 0.10000E+01 volume 0.22818E+01 ppm1 7.768 ppm2 7.100
ASSI { 351}
(( segid "PROT" and resid 118 and name HN ))
(( segid "PROT" and resid 116 and name HA ))
2.800 2.000 2.000 peak 351 weight 0.10000E+01 volume 0.48649E+01 ppm1 7.770 ppm2 4.308
ASSI { 361}
(( segid "PROT" and resid 118 and name HN ))
(( segid "PROT" and resid 116 and name HG12))
3.500 3.100 2.000 peak 361 weight 0.10000E+01 volume 0.14512E+01 ppm1 7.771 ppm2 0.923
ASSI { 411}
(( segid "PROT" and resid 28 and name HN ))
(( segid "PROT" and resid 28 and name HA ))
2.600 1.700 1.700 peak 411 weight 0.10000E+01 volume 0.75737E+01 ppm1 7.561 ppm2 4.010
ASSI { 421}
(( segid "PROT" and resid 28 and name HN ))
(( segid "PROT" and resid 25 and name HA ))
3.100 2.400 2.400 peak 421 weight 0.10000E+01 volume 0.30883E+01 ppm1 7.564 ppm2 3.858
ASSI { 431}
(( segid "PROT" and resid 28 and name HN ))
(( segid "PROT" and resid 28 and name HB1 ))
2.600 1.700 1.700 peak 431 weight 0.10000E+01 volume 0.85703E+01 ppm1 7.562 ppm2 2.994
ASSI { 441}
(( segid "PROT" and resid 28 and name HN ))
(( segid "PROT" and resid 26 and name HD1 ))
3.500 3.100 2.000 peak 441 weight 0.10000E+01 volume 0.13903E+01 ppm1 7.562 ppm2 1.839
ASSI { 451}
(( segid "PROT" and resid 28 and name HN ))
(( segid "PROT" and resid 31 and name HB% ))
2.800 2.000 2.000 peak 451 weight 0.10000E+01 volume 0.53325E+01 ppm1 7.561 ppm2 1.734
ASSI { 461}
(( segid "PROT" and resid 28 and name HN ))
(( segid "PROT" and resid 102 and name HD1% ))
3.000 2.200 2.200 peak 461 weight 0.10000E+01 volume 0.32864E+01 ppm1 7.561 ppm2 0.733
ASSI { 471}
(( segid "PROT" and resid 28 and name HN ))
(( segid "PROT" and resid 27 and name HA ))
3.100 2.400 2.400 peak 471 weight 0.10000E+01 volume 0.28492E+01 ppm1 7.559 ppm2 4.462
ASSI { 481}
(( segid "PROT" and resid 28 and name HN ))
(( segid "PROT" and resid 28 and name HB2 ))
2.500 1.600 1.600 peak 481 weight 0.10000E+01 volume 0.92253E+01 ppm1 7.558 ppm2 2.796
ASSI { 491}
(( segid "PROT" and resid 51 and name HN ))
(( segid "PROT" and resid 51 and name HD1 ))
3.300 2.700 2.200 peak 491 weight 0.10000E+01 volume 0.18829E+01 ppm1 7.766 ppm2 3.005
ASSI { 501}
(( segid "PROT" and resid 118 and name HN ))
(( segid "PROT" and resid 118 and name HG1 ))
2.300 1.300 1.300 peak 501 weight 0.10000E+01 volume 0.16392E+02 ppm1 7.764 ppm2 1.373
ASSI { 511}
(( segid "PROT" and resid 51 and name HN ))
(( segid "PROT" and resid 52 and name HN ))
2.500 1.600 1.600 peak 511 weight 0.10000E+01 volume 0.10570E+02 ppm1 7.756 ppm2 8.424
ASSI { 521}
(( segid "PROT" and resid 51 and name HN ))
(( segid "PROT" and resid 50 and name HA ))
2.100 1.100 1.100 peak 521 weight 0.10000E+01 volume 0.28178E+02 ppm1 7.762 ppm2 3.931
ASSI { 531}
(( segid "PROT" and resid 51 and name HN ))
(( segid "PROT" and resid 51 and name HB2 ))
2.500 1.600 1.600 peak 531 weight 0.10000E+01 volume 0.10172E+02 ppm1 7.757 ppm2 1.182
ASSI { 541}
(( segid "PROT" and resid 51 and name HN ))
(( segid "PROT" and resid 50 and name HD1% ))

```

2.900	2.100	2.100	peak	541	weight	0.10000E+01	volume	0.41637E+01	ppm1	7.756	ppm2	0.553
ASSI { 551}												
((segid "PROT" and resid 51 and name HN))												
(segid "PROT" and resid 50 and name HG2%)												
2.900	2.100	2.100	peak	551	weight	0.10000E+01	volume	0.43238E+01	ppm1	7.755	ppm2	0.397
ASSI { 561}												
((segid "PROT" and resid 51 and name HN))												
((segid "PROT" and resid 50 and name HN))												
3.200	2.600	2.300	peak	561	weight	0.10000E+01	volume	0.22364E+01	ppm1	7.752	ppm2	7.979
ASSI { 571}												
((segid "PROT" and resid 38 and name HN))												
((segid "PROT" and resid 37 and name HA))												
2.600	1.700	1.700	peak	571	weight	0.10000E+01	volume	0.79316E+01	ppm1	8.336	ppm2	4.242
ASSI { 581}												
((segid "PROT" and resid 38 and name HN))												
((segid "PROT" and resid 38 and name HA))												
3.200	2.600	2.300	peak	581	weight	0.10000E+01	volume	0.24318E+01	ppm1	8.334	ppm2	3.475
ASSI { 591}												
((segid "PROT" and resid 38 and name HN))												
((segid "PROT" and resid 37 and name HB1))												
3.100	2.400	2.400	peak	591	weight	0.10000E+01	volume	0.26287E+01	ppm1	8.336	ppm2	2.361
ASSI { 601}												
((segid "PROT" and resid 38 and name HN))												
((segid "PROT" and resid 38 and name HB))												
2.800	2.000	2.000	peak	601	weight	0.10000E+01	volume	0.49359E+01	ppm1	8.339	ppm2	1.058
ASSI { 611}												
((segid "PROT" and resid 38 and name HN))												
(segid "PROT" and resid 38 and name HG1%)												
2.700	1.800	1.800	peak	611	weight	0.10000E+01	volume	0.67420E+01	ppm1	8.336	ppm2	0.469
ASSI { 621}												
((segid "PROT" and resid 38 and name HN))												
((segid "PROT" and resid 37 and name HB2))												
3.500	3.100	2.000	peak	621	weight	0.10000E+01	volume	0.14362E+01	ppm1	8.331	ppm2	1.685
ASSI { 631}												
((segid "PROT" and resid 38 and name HN))												
(segid "PROT" and resid 38 and name HG2%)												
3.300	2.700	2.200	peak	631	weight	0.10000E+01	volume	0.17918E+01	ppm1	8.328	ppm2	-0.027
ASSI { 651}												
((segid "PROT" and resid 61 and name HN))												
((segid "PROT" and resid 60 and name HB1))												
3.100	2.400	2.400	peak	651	weight	0.10000E+01	volume	0.30032E+01	ppm1	8.163	ppm2	4.212
ASSI { 661}												
((segid "PROT" and resid 61 and name HN))												
((segid "PROT" and resid 61 and name HA))												
2.600	1.700	1.700	peak	661	weight	0.10000E+01	volume	0.77544E+01	ppm1	8.162	ppm2	4.060
ASSI { 671}												
((segid "PROT" and resid 61 and name HN))												
((segid "PROT" and resid 58 and name HA))												
3.300	2.700	2.200	peak	671	weight	0.10000E+01	volume	0.19907E+01	ppm1	8.162	ppm2	3.866
ASSI { 681}												
((segid "PROT" and resid 61 and name HN))												
((segid "PROT" and resid 61 and name HG2))												
2.500	1.600	1.600	peak	681	weight	0.10000E+01	volume	0.10559E+02	ppm1	8.163	ppm2	2.245
ASSI { 691}												
((segid "PROT" and resid 61 and name HN))												
((segid "PROT" and resid 61 and name HB2))												
2.700	1.800	1.800	peak	691	weight	0.10000E+01	volume	0.70727E+01	ppm1	8.163	ppm2	2.089
ASSI { 701}												
((segid "PROT" and resid 61 and name HN))												
(segid "PROT" and resid 58 and name HG2%)												
3.400	2.900	2.100	peak	701	weight	0.10000E+01	volume	0.17011E+01	ppm1	8.164	ppm2	1.075
ASSI { 711}												
((segid "PROT" and resid 61 and name HN))												
((segid "PROT" and resid 62 and name HN))												
2.700	1.800	1.800	peak	711	weight	0.10000E+01	volume	0.60705E+01	ppm1	8.161	ppm2	8.378
ASSI { 721}												
((segid "PROT" and resid 61 and name HN))												
((segid "PROT" and resid 60 and name HA))												
3.100	2.400	2.400	peak	721	weight	0.10000E+01	volume	0.27541E+01	ppm1	8.158	ppm2	4.417
ASSI { 731}												
((segid "PROT" and resid 61 and name HN))												
((segid "PROT" and resid 61 and name HG1))												
2.700	1.800	1.800	peak	731	weight	0.10000E+01	volume	0.60769E+01	ppm1	8.160	ppm2	2.388
ASSI { 741}												
((segid "PROT" and resid 117 and name HN))												
((segid "PROT" and resid 118 and name HN))												
3.000	2.200	2.200	peak	741	weight	0.10000E+01	volume	0.33860E+01	ppm1	8.278	ppm2	7.777
ASSI { 751}												
((segid "PROT" and resid 117 and name HN))												
((segid "PROT" and resid 116 and name HN))												
3.100	2.400	2.400	peak	751	weight	0.10000E+01	volume	0.30296E+01	ppm1	8.276	ppm2	7.477
ASSI { 761}												
((segid "PROT" and resid 117 and name HN))												
((segid "PROT" and resid 117 and name HA))												
2.800	2.000	2.000	peak	761	weight	0.10000E+01	volume	0.56966E+01	ppm1	8.279	ppm2	4.584
ASSI { 771}												
((segid "PROT" and resid 117 and name HN))												
((segid "PROT" and resid 115 and name HA))												
2.400	2.400	2.100	peak	771	weight	0.10000E+01	volume	0.11755E+02	ppm1	8.279	ppm2	4.253


```

ASSI { 791}
  (( segid "PROT" and resid 117 and name HN ))
  (( segid "PROT" and resid 117 and name HB1 ))
  3.100 2.400 2.400 peak 791 weight 0.10000E+01 volume 0.30574E+01 ppm1 8.279 ppm2 2.708
ASSI { 801}
  (( segid "PROT" and resid 117 and name HN ))
  (( segid "PROT" and resid 117 and name HB2 ))
  2.800 2.000 2.000 peak 801 weight 0.10000E+01 volume 0.52392E+01 ppm1 8.276 ppm2 2.564
ASSI { 811}
  (( segid "PROT" and resid 117 and name HN ))
  (( segid "PROT" and resid 116 and name HB ))
  2.800 2.000 2.000 peak 811 weight 0.10000E+01 volume 0.47120E+01 ppm1 8.279 ppm2 1.829
ASSI { 821}
  (( segid "PROT" and resid 117 and name HN ))
  (( segid "PROT" and resid 111 and name HG2 ))
  3.500 3.100 2.000 peak 821 weight 0.10000E+01 volume 0.13421E+01 ppm1 8.279 ppm2 1.309
ASSI { 831}
  (( segid "PROT" and resid 117 and name HN ))
  (( segid "PROT" and resid 116 and name HD1% ))
  3.100 2.400 2.400 peak 831 weight 0.10000E+01 volume 0.30974E+01 ppm1 8.279 ppm2 0.827
ASSI { 841}
  (( segid "PROT" and resid 6 and name HN ))
  (( segid "PROT" and resid 6 and name HB2 ))
  3.500 3.100 2.000 peak 841 weight 0.10000E+01 volume 0.12891E+01 ppm1 8.404 ppm2 1.751
ASSI { 851}
  (( segid "PROT" and resid 6 and name HN ))
  (( segid "PROT" and resid 5 and name HA ))
  3.100 2.400 2.400 peak 851 weight 0.10000E+01 volume 0.28648E+01 ppm1 8.391 ppm2 4.447
ASSI { 871}
  (( segid "PROT" and resid 50 and name HN ))
  (( segid "PROT" and resid 49 and name HN ))
  2.300 1.300 1.300 peak 871 weight 0.10000E+01 volume 0.15808E+02 ppm1 7.961 ppm2 7.117
ASSI { 881}
  (( segid "PROT" and resid 50 and name HN ))
  (( segid "PROT" and resid 48 and name HA ))
  2.800 2.000 2.000 peak 881 weight 0.10000E+01 volume 0.48582E+01 ppm1 7.960 ppm2 4.097
ASSI { 891}
  (( segid "PROT" and resid 50 and name HN ))
  (( segid "PROT" and resid 50 and name HA ))
  2.900 2.100 2.100 peak 891 weight 0.10000E+01 volume 0.39149E+01 ppm1 7.959 ppm2 3.931
ASSI { 901}
  (( segid "PROT" and resid 50 and name HN ))
  (( segid "PROT" and resid 49 and name HB ))
  2.800 2.000 2.000 peak 901 weight 0.10000E+01 volume 0.50087E+01 ppm1 7.960 ppm2 1.908
ASSI { 911}
  (( segid "PROT" and resid 50 and name HN ))
  (( segid "PROT" and resid 50 and name HB ))
  2.600 1.700 1.700 peak 911 weight 0.10000E+01 volume 0.88755E+01 ppm1 7.961 ppm2 1.220
ASSI { 921}
  (( segid "PROT" and resid 50 and name HN ))
  (( segid "PROT" and resid 49 and name HG2% ))
  2.800 2.000 2.000 peak 921 weight 0.10000E+01 volume 0.51983E+01 ppm1 7.961 ppm2 0.935
ASSI { 931}
  (( segid "PROT" and resid 50 and name HN ))
  (( segid "PROT" and resid 50 and name HG11 ))
  2.900 2.100 2.100 peak 931 weight 0.10000E+01 volume 0.42899E+01 ppm1 7.959 ppm2 0.807
ASSI { 941}
  (( segid "PROT" and resid 50 and name HN ))
  (( segid "PROT" and resid 50 and name HD1% ))
  2.900 2.100 2.100 peak 941 weight 0.10000E+01 volume 0.39098E+01 ppm1 7.963 ppm2 0.549
ASSI { 951}
  (( segid "PROT" and resid 50 and name HN ))
  (( segid "PROT" and resid 50 and name HG2% ))
  2.900 2.100 2.100 peak 951 weight 0.10000E+01 volume 0.39287E+01 ppm1 7.961 ppm2 0.395
ASSI { 961}
  (( segid "PROT" and resid 50 and name HN ))
  (( segid "PROT" and resid 50 and name HG12 ))
  3.200 2.600 2.300 peak 961 weight 0.10000E+01 volume 0.21710E+01 ppm1 7.961 ppm2 0.162
ASSI { 971}
  (( segid "PROT" and resid 50 and name HN ))
  (( segid "PROT" and resid 46 and name HA ))
  3.500 3.100 2.000 peak 971 weight 0.10000E+01 volume 0.12530E+01 ppm1 7.957 ppm2 3.478
ASSI { 981}
  (( segid "PROT" and resid 7 and name HN ))
  (( segid "PROT" and resid 7 and name HB1 ))
  2.900 2.100 2.100 peak 981 weight 0.10000E+01 volume 0.42394E+01 ppm1 8.324 ppm2 2.043
ASSI { 991}
  (( segid "PROT" and resid 7 and name HN ))
  (( segid "PROT" and resid 7 and name HA ))
  2.800 2.000 2.000 peak 991 weight 0.10000E+01 volume 0.53094E+01 ppm1 8.324 ppm2 4.561
ASSI { 1001}
  (( segid "PROT" and resid 7 and name HN ))
  (( segid "PROT" and resid 6 and name HA ))
  2.400 1.400 1.400 peak 1001 weight 0.10000E+01 volume 0.13634E+02 ppm1 8.324 ppm2 4.372
ASSI { 1011}
  (( segid "PROT" and resid 7 and name HN ))
  (( segid "PROT" and resid 8 and name HD2 ))
  3.600 3.200 1.900 peak 1011 weight 0.10000E+01 volume 0.12154E+01 ppm1 8.322 ppm2 3.707
ASSI { 1021}

```

```

(( segid "PROT" and resid 7 and name HN ))
(( segid "PROT" and resid 7 and name HG1 ))
2.900 2.100 2.100 peak 1021 weight 0.10000E+01 volume 0.40289E+01 ppm1 8.321 ppm2 2.294
ASSI { 1031}
(( segid "PROT" and resid 7 and name HN ))
(( segid "PROT" and resid 7 and name HB2 ))
2.600 1.700 1.700 peak 1031 weight 0.10000E+01 volume 0.80771E+01 ppm1 8.323 ppm2 1.912
ASSI { 1041}
(( segid "PROT" and resid 102 and name HN ))
(( segid "PROT" and resid 101 and name HN ))
2.600 1.700 1.700 peak 1041 weight 0.10000E+01 volume 0.88803E+01 ppm1 8.518 ppm2 8.030
ASSI { 1051}
(( segid "PROT" and resid 102 and name HN ))
(( segid "PROT" and resid 105 and name HN ))
3.400 2.900 2.100 peak 1051 weight 0.10000E+01 volume 0.16580E+01 ppm1 8.517 ppm2 7.932
ASSI { 1061}
(( segid "PROT" and resid 102 and name HN ))
(( segid "PROT" and resid 98 and name HA ))
3.500 3.100 2.000 peak 1061 weight 0.10000E+01 volume 0.13507E+01 ppm1 8.515 ppm2 4.197
ASSI { 1071}
(( segid "PROT" and resid 102 and name HN ))
(( segid "PROT" and resid 99 and name HA ))
3.300 2.700 2.200 peak 1071 weight 0.10000E+01 volume 0.17668E+01 ppm1 8.518 ppm2 3.874
ASSI { 1081}
(( segid "PROT" and resid 102 and name HN ))
(( segid "PROT" and resid 102 and name HA ))
2.800 2.000 2.000 peak 1081 weight 0.10000E+01 volume 0.49359E+01 ppm1 8.516 ppm2 3.686
ASSI { 1111}
(( segid "PROT" and resid 102 and name HN ))
(( segid "PROT" and resid 102 and name HG ))
3.100 2.400 2.400 peak 1111 weight 0.10000E+01 volume 0.25668E+01 ppm1 8.517 ppm2 1.554
ASSI { 1121}
(( segid "PROT" and resid 102 and name HN ))
(( segid "PROT" and resid 102 and name HB1 ))
2.800 2.000 2.000 peak 1121 weight 0.10000E+01 volume 0.54544E+01 ppm1 8.516 ppm2 1.434
ASSI { 1131}
(( segid "PROT" and resid 102 and name HN ))
(( segid "PROT" and resid 102 and name HB2 ))
2.600 1.700 1.700 peak 1131 weight 0.10000E+01 volume 0.74477E+01 ppm1 8.516 ppm2 1.232
ASSI { 1141}
(( segid "PROT" and resid 102 and name HN ))
(( segid "PROT" and resid 101 and name HG2% ))
2.900 2.100 2.100 peak 1141 weight 0.10000E+01 volume 0.42361E+01 ppm1 8.517 ppm2 1.002
ASSI { 1151}
(( segid "PROT" and resid 102 and name HN ))
(( segid "PROT" and resid 102 and name HD1% ))
2.900 2.100 2.100 peak 1151 weight 0.10000E+01 volume 0.42645E+01 ppm1 8.517 ppm2 0.732
ASSI { 1161}
(( segid "PROT" and resid 102 and name HN ))
(( segid "PROT" and resid 104 and name HN ))
3.400 2.900 2.100 peak 1161 weight 0.10000E+01 volume 0.15534E+01 ppm1 8.511 ppm2 7.182
ASSI { 1171}
(( segid "PROT" and resid 103 and name HN ))
(( segid "PROT" and resid 102 and name HN ))
2.900 2.100 2.100 peak 1171 weight 0.10000E+01 volume 0.42887E+01 ppm1 8.040 ppm2 8.466
ASSI { 1191}
(( segid "PROT" and resid 46 and name HN ))
(( segid "PROT" and resid 43 and name HA ))
3.400 2.900 2.100 peak 1191 weight 0.10000E+01 volume 0.15537E+01 ppm1 8.047 ppm2 4.931
ASSI { 1201}
(( segid "PROT" and resid 46 and name HN ))
(( segid "PROT" and resid 44 and name HA ))
3.400 2.900 2.100 peak 1201 weight 0.10000E+01 volume 0.15220E+01 ppm1 8.041 ppm2 4.522
ASSI { 1221}
(( segid "PROT" and resid 46 and name HN ))
(( segid "PROT" and resid 46 and name HA ))
2.800 2.000 2.000 peak 1221 weight 0.10000E+01 volume 0.52605E+01 ppm1 8.039 ppm2 3.484
ASSI { 1231}
(( segid "PROT" and resid 103 and name HN ))
(( segid "PROT" and resid 103 and name HA ))
3.600 3.200 1.900 peak 1231 weight 0.10000E+01 volume 0.11229E+01 ppm1 8.043 ppm2 3.216
ASSI { 1241}
(( segid "PROT" and resid 46 and name HN ))
(( segid "PROT" and resid 46 and name HB1 ))
2.600 1.700 1.700 peak 1241 weight 0.10000E+01 volume 0.84467E+01 ppm1 8.040 ppm2 2.731
ASSI { 1251}
(( segid "PROT" and resid 46 and name HN ))
(( segid "PROT" and resid 46 and name HB2 ))
2.600 1.700 1.700 peak 1251 weight 0.10000E+01 volume 0.81520E+01 ppm1 8.039 ppm2 2.395
ASSI { 1261}
(( segid "PROT" and resid 46 and name HN ))
(( segid "PROT" and resid 43 and name HB% ))
2.900 2.100 2.100 peak 1261 weight 0.10000E+01 volume 0.42142E+01 ppm1 8.040 ppm2 0.962
ASSI { 1271}
(( segid "PROT" and resid 46 and name HN ))
(( segid "PROT" and resid 48 and name HN ))
3.400 2.900 2.100 peak 1271 weight 0.10000E+01 volume 0.16926E+01 ppm1 8.036 ppm2 7.723
ASSI { 1321}
(( segid "PROT" and resid 58 and name HN ))

```

```

(( segid "PROT" and resid 59 and name HN ))
2.900 2.100 2.100 peak 1321 weight 0.10000E+01 volume 0.38254E+01 ppm1 9.442 ppm2 7.886
ASSI { 1331}
(( segid "PROT" and resid 58 and name HN ))
(( segid "PROT" and resid 58 and name HB ))
3.000 2.200 2.200 peak 1331 weight 0.10000E+01 volume 0.32050E+01 ppm1 9.442 ppm2 4.084
ASSI { 1341}
(( segid "PROT" and resid 58 and name HN ))
(( segid "PROT" and resid 58 and name HG2*))
3.200 2.600 2.300 peak 1341 weight 0.10000E+01 volume 0.25336E+01 ppm1 9.442 ppm2 1.074
ASSI { 1351}
(( segid "PROT" and resid 58 and name HN ))
(( segid "PROT" and resid 37 and name HA ))
3.400 2.900 2.100 peak 1351 weight 0.10000E+01 volume 0.16753E+01 ppm1 9.442 ppm2 4.206
ASSI { 1361}
(( segid "PROT" and resid 102 and name HN ))
(( segid "PROT" and resid 98 and name HB2 ))
3.600 3.200 1.900 peak 1361 weight 0.10000E+01 volume 0.11010E+01 ppm1 8.501 ppm2 3.051
ASSI { 1371}
(( segid "PROT" and resid 111 and name HN ))
(( segid "PROT" and resid 112 and name HN ))
2.500 1.600 1.600 peak 1371 weight 0.10000E+01 volume 0.10907E+02 ppm1 7.568 ppm2 8.068
ASSI { 1391}
(( segid "PROT" and resid 111 and name HN ))
(( segid "PROT" and resid 111 and name HA ))
2.600 1.700 1.700 peak 1391 weight 0.10000E+01 volume 0.76380E+01 ppm1 7.569 ppm2 4.066
ASSI { 1401}
(( segid "PROT" and resid 111 and name HN ))
(( segid "PROT" and resid 107 and name HA ))
3.000 2.200 2.200 peak 1401 weight 0.10000E+01 volume 0.36812E+01 ppm1 7.567 ppm2 3.835
ASSI { 1411}
(( segid "PROT" and resid 111 and name HN ))
(( segid "PROT" and resid 112 and name HB1 ))
3.300 2.700 2.200 peak 1411 weight 0.10000E+01 volume 0.18701E+01 ppm1 7.568 ppm2 2.073
ASSI { 1421}
(( segid "PROT" and resid 111 and name HN ))
(( segid "PROT" and resid 111 and name HB1 ))
2.600 1.700 1.700 peak 1421 weight 0.10000E+01 volume 0.90750E+01 ppm1 7.568 ppm2 1.875
ASSI { 1431}
(( segid "PROT" and resid 111 and name HN ))
(( segid "PROT" and resid 111 and name HD1 ))
3.100 2.400 2.400 peak 1431 weight 0.10000E+01 volume 0.27225E+01 ppm1 7.569 ppm2 1.650
ASSI { 1441}
(( segid "PROT" and resid 111 and name HN ))
(( segid "PROT" and resid 111 and name HG1 ))
3.000 2.200 2.200 peak 1441 weight 0.10000E+01 volume 0.32606E+01 ppm1 7.568 ppm2 1.416
ASSI { 1451}
(( segid "PROT" and resid 111 and name HN ))
(( segid "PROT" and resid 111 and name HG2 ))
3.100 2.400 2.400 peak 1451 weight 0.10000E+01 volume 0.27421E+01 ppm1 7.568 ppm2 1.322
ASSI { 1471}
(( segid "PROT" and resid 111 and name HN ))
(( segid "PROT" and resid 110 and name HD1*))
3.300 2.700 2.200 peak 1471 weight 0.10000E+01 volume 0.17681E+01 ppm1 7.568 ppm2 0.543
ASSI { 1481}
(( segid "PROT" and resid 111 and name HN ))
(( segid "PROT" and resid 108 and name HA ))
3.200 2.600 2.300 peak 1481 weight 0.10000E+01 volume 0.21677E+01 ppm1 7.565 ppm2 4.202
ASSI { 1491}
(( segid "PROT" and resid 111 and name HN ))
(( segid "PROT" and resid 112 and name HG1 ))
3.500 3.100 2.000 peak 1491 weight 0.10000E+01 volume 0.12577E+01 ppm1 7.560 ppm2 2.363
ASSI { 1501}
(( segid "PROT" and resid 111 and name HN ))
(( segid "PROT" and resid 111 and name HB2 ))
2.400 1.400 1.400 peak 1501 weight 0.10000E+01 volume 0.13622E+02 ppm1 7.567 ppm2 1.761
ASSI { 1511}
(( segid "PROT" and resid 111 and name HN ))
(( segid "PROT" and resid 110 and name HG12*))
3.000 2.200 2.200 peak 1511 weight 0.10000E+01 volume 0.37474E+01 ppm1 7.567 ppm2 1.074
ASSI { 1521}
(( segid "PROT" and resid 111 and name HN ))
(( segid "PROT" and resid 110 and name HG2*))
3.000 2.200 2.200 peak 1521 weight 0.10000E+01 volume 0.32871E+01 ppm1 7.566 ppm2 0.665
ASSI { 1531}
(( segid "PROT" and resid 58 and name HN ))
(( segid "PROT" and resid 56 and name HB2 ))
3.400 2.900 2.100 peak 1531 weight 0.10000E+01 volume 0.16528E+01 ppm1 9.448 ppm2 1.432
ASSI { 1551}
(( segid "PROT" and resid 58 and name HN ))
(( segid "PROT" and resid 58 and name HA ))
3.000 2.200 2.200 peak 1551 weight 0.10000E+01 volume 0.32345E+01 ppm1 9.443 ppm2 3.856
ASSI { 1571}
(( segid "PROT" and resid 58 and name HN ))
(( segid "PROT" and resid 55 and name HB1 ))
3.000 2.200 2.200 peak 1571 weight 0.10000E+01 volume 0.37144E+01 ppm1 9.443 ppm2 2.375
ASSI { 1581}
(( segid "PROT" and resid 58 and name HN ))
(( segid "PROT" and resid 59 and name HB1 ))

```

```

3.400    2.900    2.100 peak 1581 weight 0.10000E+01 volume 0.16873E+01 ppm1 9.445 ppm2 2.167
ASSI { 1621}
(( segid "PROT" and resid 10 and name HN ))
(( segid "PROT" and resid 9 and name HG1 ))
3.600    3.200    1.900 peak 1621 weight 0.10000E+01 volume 0.11241E+01 ppm1 8.310 ppm2 1.649
ASSI { 1631}
(( segid "PROT" and resid 10 and name HN ))
(( segid "PROT" and resid 10 and name HA ))
3.000    2.200    2.200 peak 1631 weight 0.10000E+01 volume 0.35515E+01 ppm1 8.304 ppm2 4.893
ASSI { 1641}
(( segid "PROT" and resid 10 and name HN ))
(( segid "PROT" and resid 8 and name HA ))
3.400    2.900    2.100 peak 1641 weight 0.10000E+01 volume 0.17142E+01 ppm1 8.301 ppm2 4.437
ASSI { 1651}
(( segid "PROT" and resid 10 and name HN ))
(( segid "PROT" and resid 9 and name HA ))
2.500    1.600    1.600 peak 1651 weight 0.10000E+01 volume 0.10059E+02 ppm1 8.305 ppm2 4.337
ASSI { 1671}
(( segid "PROT" and resid 10 and name HN ))
(( segid "PROT" and resid 11 and name HD1 ))
3.500    3.100    2.000 peak 1671 weight 0.10000E+01 volume 0.13217E+01 ppm1 8.303 ppm2 3.874
ASSI { 1681}
(( segid "PROT" and resid 10 and name HN ))
(( segid "PROT" and resid 10 and name HB1 ))
2.900    2.100    2.100 peak 1681 weight 0.10000E+01 volume 0.41755E+01 ppm1 8.305 ppm2 2.768
ASSI { 1691}
(( segid "PROT" and resid 10 and name HN ))
(( segid "PROT" and resid 10 and name HB2 ))
2.800    2.000    2.000 peak 1691 weight 0.10000E+01 volume 0.49103E+01 ppm1 8.306 ppm2 2.707
ASSI { 1701}
(( segid "PROT" and resid 10 and name HN ))
(( segid "PROT" and resid 13 and name HB1 ))
3.400    2.900    2.100 peak 1701 weight 0.10000E+01 volume 0.15663E+01 ppm1 8.307 ppm2 2.166
ASSI { 1711}
(( segid "PROT" and resid 10 and name HN ))
(( segid "PROT" and resid 9 and name HB1 ))
3.400    2.900    2.100 peak 1711 weight 0.10000E+01 volume 0.17647E+01 ppm1 8.308 ppm2 1.864
ASSI { 1731}
(( segid "PROT" and resid 43 and name HN ))
(( segid "PROT" and resid 44 and name HD1 ))
3.500    3.100    2.000 peak 1731 weight 0.10000E+01 volume 0.12797E+01 ppm1 7.180 ppm2 3.801
ASSI { 1741}
(( segid "PROT" and resid 43 and name HN ))
(( segid "PROT" and resid 39 and name HB2 ))
3.500    3.100    2.000 peak 1741 weight 0.10000E+01 volume 0.13282E+01 ppm1 7.188 ppm2 1.905
ASSI { 1751}
(( segid "PROT" and resid 43 and name HN ))
(( segid "PROT" and resid 43 and name HA ))
3.100    2.400    2.400 peak 1751 weight 0.10000E+01 volume 0.26725E+01 ppm1 7.178 ppm2 4.963
ASSI { 1761}
(( segid "PROT" and resid 43 and name HN ))
(( segid "PROT" and resid 42 and name HA ))
3.200    2.600    2.300 peak 1761 weight 0.10000E+01 volume 0.23728E+01 ppm1 7.181 ppm2 4.472
ASSI { 1771}
(( segid "PROT" and resid 43 and name HN ))
(( segid "PROT" and resid 41 and name HA ))
3.300    2.700    2.200 peak 1771 weight 0.10000E+01 volume 0.19062E+01 ppm1 7.179 ppm2 4.078
ASSI { 1781}
(( segid "PROT" and resid 43 and name HN ))
(( segid "PROT" and resid 44 and name HD2 ))
3.300    2.700    2.200 peak 1781 weight 0.10000E+01 volume 0.17857E+01 ppm1 7.180 ppm2 3.546
ASSI { 1791}
(( segid "PROT" and resid 43 and name HN ))
(( segid "PROT" and resid 42 and name HB1 ))
3.300    2.700    2.200 peak 1791 weight 0.10000E+01 volume 0.18305E+01 ppm1 7.180 ppm2 2.196
ASSI { 1801}
(( segid "PROT" and resid 43 and name HN ))
(( segid "PROT" and resid 43 and name HB2 ))
2.700    1.800    1.800 peak 1801 weight 0.10000E+01 volume 0.58026E+01 ppm1 7.180 ppm2 0.964
ASSI { 1811}
(( segid "PROT" and resid 43 and name HN ))
(( segid "PROT" and resid 38 and name HG2 ))
3.500    3.100    2.000 peak 1811 weight 0.10000E+01 volume 0.13977E+01 ppm1 7.183 ppm2 -0.019
ASSI { 1821}
(( segid "PROT" and resid 43 and name HN ))
(( segid "PROT" and resid 42 and name HB2 ))
3.400    2.900    2.100 peak 1821 weight 0.10000E+01 volume 0.17166E+01 ppm1 7.179 ppm2 2.055
ASSI { 1831}
(( segid "PROT" and resid 14 and name HN ))
(( segid "PROT" and resid 14 and name HB1 ))
2.600    1.700    1.700 peak 1831 weight 0.10000E+01 volume 0.81036E+01 ppm1 8.204 ppm2 1.862
ASSI { 1841}
(( segid "PROT" and resid 14 and name HN ))
(( segid "PROT" and resid 14 and name HB2 ))
2.700    1.800    1.800 peak 1841 weight 0.10000E+01 volume 0.69081E+01 ppm1 8.204 ppm2 1.572
ASSI { 1851}
(( segid "PROT" and resid 14 and name HN ))
(( segid "PROT" and resid 14 and name HG ))
3.000    2.200    2.200 peak 1851 weight 0.10000E+01 volume 0.31980E+01 ppm1 8.205 ppm2 1.470

```

```

ASSI { 1861}
  (( segid "PROT" and resid 14 and name HN ))
  (( segid "PROT" and resid 14 and name HD14 ))
  2.800 2.000 2.000 peak 1861 weight 0.10000E+01 volume 0.47954E+01 ppm1 8.206 ppm2 0.812
ASSI { 1881}
  (( segid "PROT" and resid 14 and name HN ))
  (( segid "PROT" and resid 11 and name HA ))
  3.200 2.600 2.300 peak 1881 weight 0.10000E+01 volume 0.22640E+01 ppm1 8.195 ppm2 4.351
ASSI { 1891}
  (( segid "PROT" and resid 14 and name HN ))
  (( segid "PROT" and resid 14 and name HA ))
  2.700 1.800 1.800 peak 1891 weight 0.10000E+01 volume 0.59973E+01 ppm1 8.201 ppm2 4.064
ASSI { 1901}
  (( segid "PROT" and resid 13 and name HN ))
  (( segid "PROT" and resid 13 and name HG1 ))
  3.000 2.200 2.200 peak 1901 weight 0.10000E+01 volume 0.37757E+01 ppm1 8.187 ppm2 2.507
ASSI { 1911}
  (( segid "PROT" and resid 13 and name HN ))
  (( segid "PROT" and resid 12 and name HB2 ))
  2.800 2.000 2.000 peak 1911 weight 0.10000E+01 volume 0.49834E+01 ppm1 8.184 ppm2 2.773
ASSI { 1921}
  (( segid "PROT" and resid 13 and name HN ))
  (( segid "PROT" and resid 12 and name HA ))
  2.000 2.000 2.500 peak 1921 weight 0.10000E+01 volume 0.40529E+02 ppm1 8.191 ppm2 4.738
ASSI { 1931}
  (( segid "PROT" and resid 13 and name HN ))
  (( segid "PROT" and resid 13 and name HA ))
  2.600 1.700 1.700 peak 1931 weight 0.10000E+01 volume 0.72316E+01 ppm1 8.189 ppm2 4.186
ASSI { 1941}
  (( segid "PROT" and resid 13 and name HN ))
  (( segid "PROT" and resid 15 and name HB2 ))
  3.500 3.100 2.000 peak 1941 weight 0.10000E+01 volume 0.14798E+01 ppm1 8.188 ppm2 3.060
ASSI { 1951}
  (( segid "PROT" and resid 13 and name HN ))
  (( segid "PROT" and resid 13 and name HB1 ))
  2.300 1.300 1.300 peak 1951 weight 0.10000E+01 volume 0.17203E+02 ppm1 8.188 ppm2 2.169
ASSI { 1971}
  (( segid "PROT" and resid 13 and name HN ))
  (( segid "PROT" and resid 13 and name HG2 ))
  2.900 2.100 2.100 peak 1971 weight 0.10000E+01 volume 0.42736E+01 ppm1 8.183 ppm2 2.406
ASSI { 1981}
  (( segid "PROT" and resid 9 and name HN ))
  (( segid "PROT" and resid 10 and name HN ))
  3.000 2.200 2.200 peak 1981 weight 0.10000E+01 volume 0.31853E+01 ppm1 8.448 ppm2 8.320
ASSI { 1991}
  (( segid "PROT" and resid 9 and name HN ))
  (( segid "PROT" and resid 7 and name HA ))
  3.200 2.600 2.300 peak 1991 weight 0.10000E+01 volume 0.21603E+01 ppm1 8.450 ppm2 4.562
ASSI { 2001}
  (( segid "PROT" and resid 9 and name HN ))
  (( segid "PROT" and resid 8 and name HA ))
  2.300 1.300 1.300 peak 2001 weight 0.10000E+01 volume 0.19003E+02 ppm1 8.447 ppm2 4.440
ASSI { 2011}
  (( segid "PROT" and resid 9 and name HN ))
  (( segid "PROT" and resid 9 and name HA ))
  2.700 1.800 1.800 peak 2011 weight 0.10000E+01 volume 0.60317E+01 ppm1 8.447 ppm2 4.335
ASSI { 2021}
  (( segid "PROT" and resid 9 and name HN ))
  (( segid "PROT" and resid 8 and name HB1 ))
  3.100 2.400 2.400 peak 2021 weight 0.10000E+01 volume 0.27796E+01 ppm1 8.445 ppm2 2.277
ASSI { 2031}
  (( segid "PROT" and resid 9 and name HN ))
  (( segid "PROT" and resid 8 and name HG1 ))
  3.400 2.900 2.100 peak 2031 weight 0.10000E+01 volume 0.16094E+01 ppm1 8.444 ppm2 2.032
ASSI { 2051}
  (( segid "PROT" and resid 9 and name HN ))
  (( segid "PROT" and resid 9 and name HG1 ))
  3.000 2.200 2.200 peak 2051 weight 0.10000E+01 volume 0.32889E+01 ppm1 8.445 ppm2 1.685
ASSI { 2061}
  (( segid "PROT" and resid 112 and name HN ))
  (( segid "PROT" and resid 108 and name HA ))
  3.200 2.600 2.300 peak 2061 weight 0.10000E+01 volume 0.22954E+01 ppm1 8.062 ppm2 4.205
ASSI { 2071}
  (( segid "PROT" and resid 112 and name HN ))
  (( segid "PROT" and resid 114 and name HN ))
  3.100 2.400 2.400 peak 2071 weight 0.10000E+01 volume 0.29684E+01 ppm1 8.062 ppm2 7.777
ASSI { 2081}
  (( segid "PROT" and resid 112 and name HN ))
  (( segid "PROT" and resid 113 and name HN ))
  2.400 1.400 1.400 peak 2081 weight 0.10000E+01 volume 0.12819E+02 ppm1 8.062 ppm2 7.594
ASSI { 2091}
  (( segid "PROT" and resid 112 and name HN ))
  (( segid "PROT" and resid 113 and name HA ))
  3.300 2.700 2.200 peak 2091 weight 0.10000E+01 volume 0.18076E+01 ppm1 8.062 ppm2 4.319
ASSI { 2101}
  (( segid "PROT" and resid 112 and name HN ))
  (( segid "PROT" and resid 112 and name HA ))
  2.400 1.400 1.400 peak 2101 weight 0.10000E+01 volume 0.12528E+02 ppm1 8.062 ppm2 4.004
ASSI { 2111}

```

```

(( segid "PROT" and resid 112 and name HN ))
(( segid "PROT" and resid 112 and name HG1 ))
2.800 2.000 2.000 peak 2111 weight 0.10000E+01 volume 0.53710E+01 ppm1 8.063 ppm2 2.367
ASSI { 2121}
(( segid "PROT" and resid 112 and name HN ))
(( segid "PROT" and resid 112 and name HG2 ))
2.900 2.100 2.100 peak 2121 weight 0.10000E+01 volume 0.39999E+01 ppm1 8.061 ppm2 2.229
ASSI { 2131}
(( segid "PROT" and resid 112 and name HN ))
(( segid "PROT" and resid 112 and name HB1 ))
2.200 1.200 1.200 peak 2131 weight 0.10000E+01 volume 0.19429E+02 ppm1 8.063 ppm2 2.082
ASSI { 2141}
(( segid "PROT" and resid 112 and name HN ))
(( segid "PROT" and resid 111 and name HB1 ))
2.600 1.700 1.700 peak 2141 weight 0.10000E+01 volume 0.76296E+01 ppm1 8.063 ppm2 1.878
ASSI { 2151}
(( segid "PROT" and resid 112 and name HN ))
(( segid "PROT" and resid 111 and name HG1 ))
2.900 2.100 2.100 peak 2151 weight 0.10000E+01 volume 0.39254E+01 ppm1 8.062 ppm2 1.400
ASSI { 2171}
(( segid "PROT" and resid 105 and name HN ))
(( segid "PROT" and resid 106 and name HN ))
2.700 1.800 1.800 peak 2171 weight 0.10000E+01 volume 0.64918E+01 ppm1 7.895 ppm2 9.143
ASSI { 2181}
(( segid "PROT" and resid 105 and name HN ))
(( segid "PROT" and resid 105 and name HB2 ))
2.600 1.700 1.700 peak 2181 weight 0.10000E+01 volume 0.82226E+01 ppm1 7.897 ppm2 3.069
ASSI { 2191}
(( segid "PROT" and resid 109 and name HN ))
(( segid "PROT" and resid 112 and name HN ))
2.400 2.400 2.100 peak 2191 weight 0.10000E+01 volume 0.13989E+02 ppm1 7.966 ppm2 8.061
ASSI { 2201}
(( segid "PROT" and resid 105 and name HN ))
(( segid "PROT" and resid 107 and name HN ))
3.500 3.100 2.000 peak 2201 weight 0.10000E+01 volume 0.13375E+01 ppm1 7.906 ppm2 8.386
ASSI { 2221}
(( segid "PROT" and resid 105 and name HN ))
(( segid "PROT" and resid 104 and name HN ))
2.500 1.600 1.600 peak 2221 weight 0.10000E+01 volume 0.98549E+01 ppm1 7.898 ppm2 7.183
ASSI { 2231}
(( segid "PROT" and resid 105 and name HN ))
(( segid "PROT" and resid 105 and name HA ))
2.800 2.000 2.000 peak 2231 weight 0.10000E+01 volume 0.54794E+01 ppm1 7.898 ppm2 4.341
ASSI { 2241}
(( segid "PROT" and resid 105 and name HN ))
(( segid "PROT" and resid 101 and name HA ))
2.900 2.100 2.100 peak 2241 weight 0.10000E+01 volume 0.40771E+01 ppm1 7.899 ppm2 3.693
ASSI { 2251}
(( segid "PROT" and resid 105 and name HN ))
(( segid "PROT" and resid 105 and name HB1 ))
2.600 1.700 1.700 peak 2251 weight 0.10000E+01 volume 0.78556E+01 ppm1 7.897 ppm2 3.149
ASSI { 2261}
(( segid "PROT" and resid 105 and name HN ))
(( segid "PROT" and resid 104 and name HB1 ))
2.600 1.700 1.700 peak 2261 weight 0.10000E+01 volume 0.79995E+01 ppm1 7.897 ppm2 1.951
ASSI { 2271}
(( segid "PROT" and resid 105 and name HN ))
(( segid "PROT" and resid 104 and name HG1 ))
3.400 2.900 2.100 peak 2271 weight 0.10000E+01 volume 0.16588E+01 ppm1 7.894 ppm2 1.538
ASSI { 2281}
(( segid "PROT" and resid 105 and name HN ))
(( segid "PROT" and resid 102 and name HD2* ))
3.200 2.600 2.300 peak 2281 weight 0.10000E+01 volume 0.22009E+01 ppm1 7.898 ppm2 0.737
ASSI { 2301}
(( segid "PROT" and resid 109 and name HN ))
(( segid "PROT" and resid 108 and name HA ))
3.100 2.400 2.400 peak 2301 weight 0.10000E+01 volume 0.25704E+01 ppm1 7.966 ppm2 4.207
ASSI { 2311}
(( segid "PROT" and resid 109 and name HN ))
(( segid "PROT" and resid 109 and name HE2 ))
3.400 2.900 2.100 peak 2311 weight 0.10000E+01 volume 0.15036E+01 ppm1 7.969 ppm2 2.462
ASSI { 2321}
(( segid "PROT" and resid 109 and name HN ))
(( segid "PROT" and resid 109 and name HG1 ))
2.600 1.700 1.700 peak 2321 weight 0.10000E+01 volume 0.78656E+01 ppm1 7.966 ppm2 0.828
ASSI { 2331}
(( segid "PROT" and resid 109 and name HN ))
(( segid "PROT" and resid 111 and name HN ))
3.100 2.400 2.400 peak 2331 weight 0.10000E+01 volume 0.27030E+01 ppm1 7.959 ppm2 7.567
ASSI { 2341}
(( segid "PROT" and resid 109 and name HN ))
(( segid "PROT" and resid 105 and name HA ))
3.400 2.900 2.100 peak 2341 weight 0.10000E+01 volume 0.15976E+01 ppm1 7.964 ppm2 4.340
ASSI { 2351}
(( segid "PROT" and resid 109 and name HN ))
(( segid "PROT" and resid 108 and name HB1 ))
2.500 1.600 1.600 peak 2351 weight 0.10000E+01 volume 0.95438E+01 ppm1 7.965 ppm2 4.004
ASSI { 2361}
(( segid "PROT" and resid 109 and name HN ))

```

```

(( segid "PROT" and resid 107 and name HA ))
3.200 2.600 2.300 peak 2361 weight 0.10000E+01 volume 0.23540E+01 ppm1 7.963 ppm2 3.853
ASSI { 2371}
(( segid "PROT" and resid 109 and name HN ))
(( segid "PROT" and resid 109 and name HB1 ))
2.600 1.700 1.700 peak 2371 weight 0.10000E+01 volume 0.85245E+01 ppm1 7.965 ppm2 1.736
ASSI { 2381}
(( segid "PROT" and resid 109 and name HN ))
(( segid "PROT" and resid 109 and name HB2 ))
2.800 2.000 2.000 peak 2381 weight 0.10000E+01 volume 0.48841E+01 ppm1 7.964 ppm2 1.564
ASSI { 2391}
(( segid "PROT" and resid 109 and name HN ))
(( segid "PROT" and resid 109 and name HD1 ))
2.900 2.100 2.100 peak 2391 weight 0.10000E+01 volume 0.42717E+01 ppm1 7.961 ppm2 1.394
ASSI { 2401}
(( segid "PROT" and resid 109 and name HN ))
(( segid "PROT" and resid 110 and name HG11))
3.400 2.900 2.100 peak 2401 weight 0.10000E+01 volume 0.15305E+01 ppm1 7.962 ppm2 1.140
ASSI { 2411}
(( segid "PROT" and resid 109 and name HN ))
(( segid "PROT" and resid 107 and name HN ))
3.600 3.200 1.900 peak 2411 weight 0.10000E+01 volume 0.11700E+01 ppm1 7.954 ppm2 8.397
ASSI { 2421}
(( segid "PROT" and resid 106 and name HN ))
(( segid "PROT" and resid 102 and name HA ))
3.400 2.900 2.100 peak 2421 weight 0.10000E+01 volume 0.16616E+01 ppm1 9.157 ppm2 3.700
ASSI { 2431}
(( segid "PROT" and resid 106 and name HN ))
(( segid "PROT" and resid 107 and name HN ))
2.800 2.000 2.000 peak 2431 weight 0.10000E+01 volume 0.54826E+01 ppm1 9.149 ppm2 8.399
ASSI { 2451}
(( segid "PROT" and resid 106 and name HN ))
(( segid "PROT" and resid 24 and name HE21))
3.300 2.700 2.200 peak 2451 weight 0.10000E+01 volume 0.17819E+01 ppm1 9.147 ppm2 7.060
ASSI { 2461}
(( segid "PROT" and resid 106 and name HN ))
(( segid "PROT" and resid 106 and name HD% ))
3.500 3.100 2.000 peak 2461 weight 0.10000E+01 volume 0.13574E+01 ppm1 9.153 ppm2 6.913
ASSI { 2471}
(( segid "PROT" and resid 106 and name HN ))
(( segid "PROT" and resid 106 and name HA ))
2.900 2.100 2.100 peak 2471 weight 0.10000E+01 volume 0.45571E+01 ppm1 9.146 ppm2 3.977
ASSI { 2481}
(( segid "PROT" and resid 106 and name HN ))
(( segid "PROT" and resid 106 and name HB1 ))
2.700 1.800 1.800 peak 2481 weight 0.10000E+01 volume 0.65451E+01 ppm1 9.149 ppm2 3.314
ASSI { 2491}
(( segid "PROT" and resid 106 and name HN ))
(( segid "PROT" and resid 106 and name HB2 ))
2.500 1.600 1.600 peak 2491 weight 0.10000E+01 volume 0.92358E+01 ppm1 9.148 ppm2 3.100
ASSI { 2511}
(( segid "PROT" and resid 106 and name HN ))
(( segid "PROT" and resid 25 and name HG1% ))
3.500 3.100 2.000 peak 2511 weight 0.10000E+01 volume 0.14013E+01 ppm1 9.149 ppm2 1.222
ASSI { 2521}
(( segid "PROT" and resid 106 and name HN ))
(( segid "PROT" and resid 104 and name HN ))
3.300 2.700 2.200 peak 2521 weight 0.10000E+01 volume 0.18869E+01 ppm1 9.146 ppm2 7.178
ASSI { 2541}
(( segid "PROT" and resid 106 and name HN ))
(( segid "PROT" and resid 105 and name HA ))
3.500 3.100 2.000 peak 2541 weight 0.10000E+01 volume 0.14398E+01 ppm1 9.142 ppm2 4.338
ASSI { 2551}
(( segid "PROT" and resid 106 and name HN ))
(( segid "PROT" and resid 104 and name HA ))
3.400 2.900 2.100 peak 2551 weight 0.10000E+01 volume 0.15238E+01 ppm1 9.143 ppm2 4.087
ASSI { 2561}
(( segid "PROT" and resid 106 and name HN ))
(( segid "PROT" and resid 102 and name HD2% ))
3.400 2.900 2.100 peak 2561 weight 0.10000E+01 volume 0.15872E+01 ppm1 9.146 ppm2 0.732
ASSI { 2571}
(( segid "PROT" and resid 84 and name HN ))
(( segid "PROT" and resid 83 and name HA ))
3.300 2.700 2.200 peak 2571 weight 0.10000E+01 volume 0.17659E+01 ppm1 8.875 ppm2 3.865
ASSI { 2581}
(( segid "PROT" and resid 84 and name HN ))
(( segid "PROT" and resid 83 and name HN ))
2.600 1.700 1.700 peak 2581 weight 0.10000E+01 volume 0.75945E+01 ppm1 8.874 ppm2 9.085
ASSI { 2601}
(( segid "PROT" and resid 84 and name HN ))
(( segid "PROT" and resid 80 and name HN ))
3.200 2.600 2.300 peak 2601 weight 0.10000E+01 volume 0.21504E+01 ppm1 8.870 ppm2 7.410
ASSI { 2611}
(( segid "PROT" and resid 84 and name HN ))
(( segid "PROT" and resid 85 and name HN ))
2.800 2.000 2.000 peak 2611 weight 0.10000E+01 volume 0.55696E+01 ppm1 8.872 ppm2 6.913
ASSI { 2621}
(( segid "PROT" and resid 84 and name HN ))
(( segid "PROT" and resid 82 and name HN ))

```

3.500	3.100	2.000	peak 2621	weight 0.10000E+01	volume 0.13351E+01	ppm1 8.872	ppm2 6.408	
ASSI { 2631}								
((segid "PROT" and resid 84 and name HN))								
((segid "PROT" and resid 84 and name HA))								
2.700	1.800	1.800	peak 2631	weight 0.10000E+01	volume 0.67391E+01	ppm1 8.874	ppm2 4.314	
ASSI { 2641}								
((segid "PROT" and resid 84 and name HN))								
((segid "PROT" and resid 83 and name HB))								
2.800	2.000	2.000	peak 2641	weight 0.10000E+01	volume 0.51222E+01	ppm1 8.874	ppm2 4.216	
ASSI { 2651}								
((segid "PROT" and resid 84 and name HN))								
((segid "PROT" and resid 80 and name HA))								
3.000	2.200	2.200	peak 2651	weight 0.10000E+01	volume 0.35702E+01	ppm1 8.873	ppm2 4.073	
ASSI { 2661}								
((segid "PROT" and resid 84 and name HN))								
((segid "PROT" and resid 81 and name HA))								
3.200	2.600	2.300	peak 2661	weight 0.10000E+01	volume 0.24366E+01	ppm1 8.875	ppm2 3.080	
ASSI { 2671}								
((segid "PROT" and resid 84 and name HN))								
((segid "PROT" and resid 84 and name HB1))								
2.800	2.000	2.000	peak 2671	weight 0.10000E+01	volume 0.49574E+01	ppm1 8.874	ppm2 2.988	
ASSI { 2681}								
((segid "PROT" and resid 84 and name HN))								
((segid "PROT" and resid 84 and name HB2))								
3.000	2.200	2.200	peak 2681	weight 0.10000E+01	volume 0.34031E+01	ppm1 8.873	ppm2 2.695	
ASSI { 2691}								
((segid "PROT" and resid 84 and name HN))								
((segid "PROT" and resid 83 and name HG2%))								
3.000	2.200	2.200	peak 2691	weight 0.10000E+01	volume 0.32105E+01	ppm1 8.872	ppm2 1.322	
ASSI { 2701}								
((segid "PROT" and resid 40 and name HN))								
((segid "PROT" and resid 40 and name HA))								
3.200	2.600	2.300	peak 2701	weight 0.10000E+01	volume 0.21281E+01	ppm1 8.066	ppm2 3.679	
ASSI { 2721}								
((segid "PROT" and resid 40 and name HN))								
((segid "PROT" and resid 42 and name HN))								
2.600	1.700	1.700	peak 2721	weight 0.10000E+01	volume 0.84529E+01	ppm1 8.061	ppm2 7.182	
ASSI { 2741}								
((segid "PROT" and resid 17 and name HN))								
((segid "PROT" and resid 15 and name HB2))								
3.300	2.700	2.200	peak 2741	weight 0.10000E+01	volume 0.20300E+01	ppm1 8.061	ppm2 3.089	
ASSI { 2751}								
((segid "PROT" and resid 40 and name HN))								
((segid "PROT" and resid 39 and name HB2))								
2.800	2.000	2.000	peak 2751	weight 0.10000E+01	volume 0.54119E+01	ppm1 8.061	ppm2 1.944	
ASSI { 2761}								
((segid "PROT" and resid 112 and name HN))								
((segid "PROT" and resid 111 and name HB2))								
2.500	1.600	1.600	peak 2761	weight 0.10000E+01	volume 0.91964E+01	ppm1 8.060	ppm2 1.761	
ASSI { 2781}								
((segid "PROT" and resid 40 and name HN))								
((segid "PROT" and resid 39 and name HG2))								
2.900	2.100	2.100	peak 2781	weight 0.10000E+01	volume 0.40049E+01	ppm1 8.058	ppm2 1.420	
ASSI { 2791}								
((segid "PROT" and resid 40 and name HN))								
((segid "PROT" and resid 41 and name HG2%))								
2.600	1.700	1.700	peak 2791	weight 0.10000E+01	volume 0.90273E+01	ppm1 8.059	ppm2 1.310	
ASSI { 2811}								
((segid "PROT" and resid 18 and name HN))								
((segid "PROT" and resid 16 and name HN))								
3.300	2.700	2.200	peak 2811	weight 0.10000E+01	volume 0.18261E+01	ppm1 8.480	ppm2 8.180	
ASSI { 2821}								
((segid "PROT" and resid 18 and name HN))								
((segid "PROT" and resid 15 and name HA))								
3.200	2.600	2.300	peak 2821	weight 0.10000E+01	volume 0.23600E+01	ppm1 8.479	ppm2 4.068	
ASSI { 2831}								
((segid "PROT" and resid 18 and name HN))								
((segid "PROT" and resid 18 and name HB2))								
3.100	2.400	2.400	peak 2831	weight 0.10000E+01	volume 0.28105E+01	ppm1 8.479	ppm2 0.321	
ASSI { 2841}								
((segid "PROT" and resid 18 and name HN))								
((segid "PROT" and resid 19 and name HN))								
2.700	1.800	1.800	peak 2841	weight 0.10000E+01	volume 0.63709E+01	ppm1 8.477	ppm2 8.560	
ASSI { 2861}								
((segid "PROT" and resid 18 and name HN))								
((segid "PROT" and resid 17 and name HB))								
2.800	2.000	2.000	peak 2861	weight 0.10000E+01	volume 0.46980E+01	ppm1 8.476	ppm2 4.264	
ASSI { 2871}								
((segid "PROT" and resid 18 and name HN))								
((segid "PROT" and resid 17 and name HA))								
3.200	2.600	2.300	peak 2871	weight 0.10000E+01	volume 0.23422E+01	ppm1 8.476	ppm2 3.944	
ASSI { 2881}								
((segid "PROT" and resid 18 and name HN))								
((segid "PROT" and resid 18 and name HA))								
3.000	2.200	2.200	peak 2881	weight 0.10000E+01	volume 0.32947E+01	ppm1 8.474	ppm2 3.286	
ASSI { 2891}								
((segid "PROT" and resid 18 and name HN))								
((segid "PROT" and resid 18 and name HG))								
2.700	1.800	1.800	peak 2891	weight 0.10000E+01	volume 0.63912E+01	ppm1 8.475	ppm2 1.680	


```

ASSI { 2901}
(( segid "PROT" and resid 18 and name HN ))
(( segid "PROT" and resid 18 and name HB1 ))
2.800 2.000 2.000 peak 2901 weight 0.10000E+01 volume 0.48006E+01 ppm1 8.475 ppm2 1.523
ASSI { 2911}
(( segid "PROT" and resid 18 and name HN ))
(( segid "PROT" and resid 17 and name HG2% ))
3.000 2.200 2.200 peak 2911 weight 0.10000E+01 volume 0.31480E+01 ppm1 8.476 ppm2 1.153
ASSI { 2931}
(( segid "PROT" and resid 18 and name HN ))
(( segid "PROT" and resid 14 and name HD2% ))
3.300 2.700 2.200 peak 2931 weight 0.10000E+01 volume 0.20785E+01 ppm1 8.476 ppm2 0.807
ASSI { 2941}
(( segid "PROT" and resid 18 and name HN ))
(( segid "PROT" and resid 18 and name HD1% ))
3.000 2.200 2.200 peak 2941 weight 0.10000E+01 volume 0.31846E+01 ppm1 8.476 ppm2 0.482
ASSI { 2951}
(( segid "PROT" and resid 18 and name HN ))
(( segid "PROT" and resid 18 and name HD2% ))
2.900 2.100 2.100 peak 2951 weight 0.10000E+01 volume 0.41898E+01 ppm1 8.475 ppm2 -0.188
ASSI { 2961}
(( segid "PROT" and resid 21 and name HN ))
(( segid "PROT" and resid 19 and name HN ))
3.100 2.400 2.400 peak 2961 weight 0.10000E+01 volume 0.28005E+01 ppm1 7.926 ppm2 8.572
ASSI { 2981}
(( segid "PROT" and resid 21 and name HN ))
(( segid "PROT" and resid 20 and name HB1 ))
2.600 1.700 1.700 peak 2981 weight 0.10000E+01 volume 0.74039E+01 ppm1 7.927 ppm2 4.077
ASSI { 2991}
(( segid "PROT" and resid 21 and name HN ))
(( segid "PROT" and resid 21 and name HB ))
2.500 1.600 1.600 peak 2991 weight 0.10000E+01 volume 0.92632E+01 ppm1 7.926 ppm2 1.918
ASSI { 3001}
(( segid "PROT" and resid 21 and name HN ))
(( segid "PROT" and resid 109 and name HB1 ))
2.600 1.700 1.700 peak 3001 weight 0.10000E+01 volume 0.77416E+01 ppm1 7.928 ppm2 1.766
ASSI { 3011}
(( segid "PROT" and resid 21 and name HN ))
(( segid "PROT" and resid 21 and name HG2% ))
2.700 1.800 1.800 peak 3011 weight 0.10000E+01 volume 0.61275E+01 ppm1 7.928 ppm2 1.014
ASSI { 3021}
(( segid "PROT" and resid 21 and name HN ))
(( segid "PROT" and resid 22 and name HN ))
2.600 1.700 1.700 peak 3021 weight 0.10000E+01 volume 0.72631E+01 ppm1 7.925 ppm2 8.852
ASSI { 3041}
(( segid "PROT" and resid 21 and name HN ))
(( segid "PROT" and resid 21 and name HA ))
2.900 2.100 2.100 peak 3041 weight 0.10000E+01 volume 0.45192E+01 ppm1 7.925 ppm2 3.776
ASSI { 3051}
(( segid "PROT" and resid 21 and name HN ))
(( segid "PROT" and resid 18 and name HA ))
3.300 2.700 2.200 peak 3051 weight 0.10000E+01 volume 0.20113E+01 ppm1 7.922 ppm2 3.290
ASSI { 3061}
(( segid "PROT" and resid 21 and name HN ))
(( segid "PROT" and resid 21 and name HD1% ))
2.900 2.100 2.100 peak 3061 weight 0.10000E+01 volume 0.38874E+01 ppm1 7.925 ppm2 0.629
ASSI { 3071}
(( segid "PROT" and resid 63 and name HN ))
(( segid "PROT" and resid 62 and name HN ))
2.800 2.000 2.000 peak 3071 weight 0.10000E+01 volume 0.52291E+01 ppm1 8.888 ppm2 8.376
ASSI { 3081}
(( segid "PROT" and resid 63 and name HN ))
(( segid "PROT" and resid 61 and name HN ))
3.300 2.700 2.200 peak 3081 weight 0.10000E+01 volume 0.18178E+01 ppm1 8.888 ppm2 8.161
ASSI { 3091}
(( segid "PROT" and resid 63 and name HN ))
(( segid "PROT" and resid 64 and name HN ))
2.700 1.800 1.800 peak 3091 weight 0.10000E+01 volume 0.60476E+01 ppm1 8.888 ppm2 8.016
ASSI { 3121}
(( segid "PROT" and resid 63 and name HN ))
(( segid "PROT" and resid 62 and name HA ))
3.400 2.900 2.100 peak 3121 weight 0.10000E+01 volume 0.15880E+01 ppm1 8.892 ppm2 3.879
ASSI { 3131}
(( segid "PROT" and resid 63 and name HN ))
(( segid "PROT" and resid 63 and name HB1 ))
2.700 1.800 1.800 peak 3131 weight 0.10000E+01 volume 0.58695E+01 ppm1 8.888 ppm2 2.320
ASSI { 3141}
(( segid "PROT" and resid 63 and name HN ))
(( segid "PROT" and resid 62 and name HB1 ))
2.800 2.000 2.000 peak 3141 weight 0.10000E+01 volume 0.46788E+01 ppm1 8.888 ppm2 2.057
ASSI { 3151}
(( segid "PROT" and resid 63 and name HN ))
(( segid "PROT" and resid 63 and name HB2 ))
2.700 1.800 1.800 peak 3151 weight 0.10000E+01 volume 0.63702E+01 ppm1 8.886 ppm2 1.941
ASSI { 3161}
(( segid "PROT" and resid 63 and name HN ))
(( segid "PROT" and resid 63 and name HG ))
3.100 2.400 2.400 peak 3161 weight 0.10000E+01 volume 0.27969E+01 ppm1 8.889 ppm2 1.820
ASSI { 3171}

```

```

(( segid "PROT" and resid 63 and name HN ))
( segid "PROT" and resid 63 and name HD2%)
3.000 2.200 2.200 peak 3171 weight 0.10000E+01 volume 0.35417E+01 ppm1 8.888 ppm2 1.060
ASSI { 3181}
(( segid "PROT" and resid 17 and name HN ))
(( segid "PROT" and resid 18 and name HN ))
2.500 1.600 1.600 peak 3181 weight 0.10000E+01 volume 0.95309E+01 ppm1 8.069 ppm2 8.473
ASSI { 3191}
(( segid "PROT" and resid 17 and name HN ))
(( segid "PROT" and resid 16 and name HN ))
2.500 1.600 1.600 peak 3191 weight 0.10000E+01 volume 0.10057E+02 ppm1 8.071 ppm2 8.187
ASSI { 3201}
(( segid "PROT" and resid 17 and name HN ))
(( segid "PROT" and resid 20 and name HN ))
3.400 2.900 2.100 peak 3201 weight 0.10000E+01 volume 0.15862E+01 ppm1 8.066 ppm2 7.549
ASSI { 3211}
(( segid "PROT" and resid 17 and name HN ))
(( segid "PROT" and resid 17 and name HB ))
2.500 1.600 1.600 peak 3211 weight 0.10000E+01 volume 0.10024E+02 ppm1 8.069 ppm2 4.262
ASSI { 3221}
(( segid "PROT" and resid 17 and name HN ))
(( segid "PROT" and resid 15 and name HA ))
2.600 1.700 1.700 peak 3221 weight 0.10000E+01 volume 0.85882E+01 ppm1 8.069 ppm2 4.044
ASSI { 3231}
(( segid "PROT" and resid 17 and name HN ))
(( segid "PROT" and resid 17 and name HA ))
2.500 1.600 1.600 peak 3231 weight 0.10000E+01 volume 0.93972E+01 ppm1 8.070 ppm2 3.947
ASSI { 3241}
(( segid "PROT" and resid 17 and name HN ))
( segid "PROT" and resid 17 and name HG2%)
2.900 2.100 2.100 peak 3241 weight 0.10000E+01 volume 0.44457E+01 ppm1 8.070 ppm2 1.153
ASSI { 3271}
(( segid "PROT" and resid 21 and name HN ))
(( segid "PROT" and resid 17 and name HA ))
3.100 2.400 2.400 peak 3271 weight 0.10000E+01 volume 0.29963E+01 ppm1 7.934 ppm2 3.946
ASSI { 3291}
(( segid "PROT" and resid 21 and name HN ))
(( segid "PROT" and resid 20 and name HA ))
3.200 2.600 2.300 peak 3291 weight 0.10000E+01 volume 0.25173E+01 ppm1 7.926 ppm2 4.300
ASSI { 3321}
(( segid "PROT" and resid 63 and name HN ))
(( segid "PROT" and resid 62 and name HG2 ))
3.200 2.600 2.300 peak 3321 weight 0.10000E+01 volume 0.23209E+01 ppm1 8.888 ppm2 0.886
ASSI { 3331}
(( segid "PROT" and resid 62 and name HN ))
(( segid "PROT" and resid 60 and name HN ))
3.500 3.100 2.000 peak 3331 weight 0.10000E+01 volume 0.13912E+01 ppm1 8.384 ppm2 7.972
ASSI { 3341}
(( segid "PROT" and resid 62 and name HN ))
(( segid "PROT" and resid 62 and name HD1 ))
3.500 3.100 2.000 peak 3341 weight 0.10000E+01 volume 0.13872E+01 ppm1 8.383 ppm2 2.575
ASSI { 3351}
(( segid "PROT" and resid 62 and name HN ))
(( segid "PROT" and resid 63 and name HB1 ))
3.500 3.100 2.000 peak 3351 weight 0.10000E+01 volume 0.14084E+01 ppm1 8.384 ppm2 2.382
ASSI { 3361}
(( segid "PROT" and resid 62 and name HN ))
(( segid "PROT" and resid 62 and name HG1 ))
3.000 2.200 2.200 peak 3361 weight 0.10000E+01 volume 0.33068E+01 ppm1 8.384 ppm2 1.733
ASSI { 3371}
(( segid "PROT" and resid 62 and name HN ))
(( segid "PROT" and resid 62 and name HG2 ))
3.200 2.600 2.300 peak 3371 weight 0.10000E+01 volume 0.23585E+01 ppm1 8.382 ppm2 0.889
ASSI { 3401}
(( segid "PROT" and resid 62 and name HN ))
(( segid "PROT" and resid 59 and name HA ))
3.400 2.900 2.100 peak 3401 weight 0.10000E+01 volume 0.16609E+01 ppm1 8.380 ppm2 4.316
ASSI { 3411}
(( segid "PROT" and resid 62 and name HN ))
(( segid "PROT" and resid 60 and name HB2 ))
3.400 2.900 2.100 peak 3411 weight 0.10000E+01 volume 0.15850E+01 ppm1 8.379 ppm2 4.058
ASSI { 3421}
(( segid "PROT" and resid 62 and name HN ))
(( segid "PROT" and resid 62 and name HA ))
3.000 2.200 2.200 peak 3421 weight 0.10000E+01 volume 0.37803E+01 ppm1 8.379 ppm2 3.882
ASSI { 3431}
(( segid "PROT" and resid 62 and name HN ))
(( segid "PROT" and resid 61 and name HB1 ))
2.900 2.100 2.100 peak 3431 weight 0.10000E+01 volume 0.46420E+01 ppm1 8.378 ppm2 2.239
ASSI { 3441}
(( segid "PROT" and resid 62 and name HN ))
(( segid "PROT" and resid 62 and name HB1 ))
2.600 1.700 1.700 peak 3441 weight 0.10000E+01 volume 0.77987E+01 ppm1 8.379 ppm2 2.071
ASSI { 3451}
(( segid "PROT" and resid 62 and name HN ))
(( segid "PROT" and resid 62 and name HB2 ))
3.000 2.200 2.200 peak 3451 weight 0.10000E+01 volume 0.36613E+01 ppm1 8.380 ppm2 1.079
ASSI { 3461}
(( segid "PROT" and resid 64 and name HN ))

```

```

(( segid "PROT" and resid 64 and name HA ))
2.500 1.600 1.600 peak 3461 weight 0.10000E+01 volume 0.92573E+01 ppm1 8.027 ppm2 4.344
ASSI { 3471}
(( segid "PROT" and resid 64 and name HN ))
(( segid "PROT" and resid 61 and name HA ))
2.800 2.000 2.000 peak 3471 weight 0.10000E+01 volume 0.51878E+01 ppm1 8.029 ppm2 4.057
ASSI { 3491}
(( segid "PROT" and resid 64 and name HN ))
(( segid "PROT" and resid 64 and name HD1 ))
2.900 2.100 2.100 peak 3491 weight 0.10000E+01 volume 0.43075E+01 ppm1 8.029 ppm2 1.803
ASSI { 3501}
(( segid "PROT" and resid 64 and name HN ))
(( segid "PROT" and resid 64 and name HG1 ))
2.900 2.100 2.100 peak 3501 weight 0.10000E+01 volume 0.45945E+01 ppm1 8.024 ppm2 1.645
ASSI { 3521}
(( segid "PROT" and resid 64 and name HN ))
(( segid "PROT" and resid 62 and name HN ))
3.500 3.100 2.000 peak 3521 weight 0.10000E+01 volume 0.12743E+01 ppm1 8.021 ppm2 8.369
ASSI { 3531}
(( segid "PROT" and resid 64 and name HN ))
(( segid "PROT" and resid 63 and name HB1 ))
2.800 2.000 2.000 peak 3531 weight 0.10000E+01 volume 0.56024E+01 ppm1 8.020 ppm2 2.320
ASSI { 3541}
(( segid "PROT" and resid 64 and name HN ))
(( segid "PROT" and resid 64 and name HB1 ))
2.200 1.200 1.200 peak 3541 weight 0.10000E+01 volume 0.19404E+02 ppm1 8.019 ppm2 2.060
ASSI { 3551}
(( segid "PROT" and resid 64 and name HN ))
(( segid "PROT" and resid 63 and name HD2% ))
3.300 2.700 2.200 peak 3551 weight 0.10000E+01 volume 0.19248E+01 ppm1 8.021 ppm2 1.055
ASSI { 3561}
(( segid "PROT" and resid 64 and name HN ))
(( segid "PROT" and resid 63 and name HD1% ))
3.200 2.600 2.300 peak 3561 weight 0.10000E+01 volume 0.25258E+01 ppm1 8.021 ppm2 0.890
ASSI { 3571}
(( segid "PROT" and resid 22 and name HN ))
(( segid "PROT" and resid 21 and name HA ))
3.400 2.900 2.100 peak 3571 weight 0.10000E+01 volume 0.16579E+01 ppm1 8.852 ppm2 3.768
ASSI { 3581}
(( segid "PROT" and resid 72 and name HN ))
(( segid "PROT" and resid 72 and name HA ))
3.000 2.200 2.200 peak 3581 weight 0.10000E+01 volume 0.37203E+01 ppm1 8.211 ppm2 4.061
ASSI { 3591}
(( segid "PROT" and resid 72 and name HN ))
(( segid "PROT" and resid 72 and name HB1 ))
2.800 2.000 2.000 peak 3591 weight 0.10000E+01 volume 0.46635E+01 ppm1 8.210 ppm2 1.925
ASSI { 3601}
(( segid "PROT" and resid 72 and name HN ))
(( segid "PROT" and resid 73 and name HN ))
3.000 2.200 2.200 peak 3601 weight 0.10000E+01 volume 0.32739E+01 ppm1 8.206 ppm2 7.441
ASSI { 3611}
(( segid "PROT" and resid 99 and name HN ))
(( segid "PROT" and resid 97 and name HA ))
3.100 2.400 2.400 peak 3611 weight 0.10000E+01 volume 0.27035E+01 ppm1 8.191 ppm2 4.210
ASSI { 3621}
(( segid "PROT" and resid 72 and name HN ))
(( segid "PROT" and resid 72 and name HB2 ))
2.800 2.000 2.000 peak 3621 weight 0.10000E+01 volume 0.47097E+01 ppm1 8.208 ppm2 1.850
ASSI { 3631}
(( segid "PROT" and resid 72 and name HN ))
(( segid "PROT" and resid 72 and name HG1 ))
3.100 2.400 2.400 peak 3631 weight 0.10000E+01 volume 0.30016E+01 ppm1 8.207 ppm2 1.539
ASSI { 3641}
(( segid "PROT" and resid 72 and name HN ))
(( segid "PROT" and resid 6 and name HG1 ))
3.300 2.700 2.200 peak 3641 weight 0.10000E+01 volume 0.18696E+01 ppm1 8.199 ppm2 1.432
ASSI { 3661}
(( segid "PROT" and resid 99 and name HN ))
(( segid "PROT" and resid 100 and name HN ))
2.600 1.700 1.700 peak 3661 weight 0.10000E+01 volume 0.76299E+01 ppm1 8.188 ppm2 8.080
ASSI { 3671}
(( segid "PROT" and resid 99 and name HN ))
(( segid "PROT" and resid 97 and name HN ))
3.400 2.900 2.100 peak 3671 weight 0.10000E+01 volume 0.17229E+01 ppm1 8.189 ppm2 7.960
ASSI { 3681}
(( segid "PROT" and resid 99 and name HN ))
(( segid "PROT" and resid 100 and name HA ))
3.600 3.200 1.900 peak 3681 weight 0.10000E+01 volume 0.12058E+01 ppm1 8.193 ppm2 4.341
ASSI { 3691}
(( segid "PROT" and resid 99 and name HN ))
(( segid "PROT" and resid 99 and name HA ))
2.900 2.100 2.100 peak 3691 weight 0.10000E+01 volume 0.45059E+01 ppm1 8.192 ppm2 3.884
ASSI { 3701}
(( segid "PROT" and resid 99 and name HN ))
(( segid "PROT" and resid 98 and name HB1 ))
3.300 2.700 2.200 peak 3701 weight 0.10000E+01 volume 0.19188E+01 ppm1 8.188 ppm2 3.381
ASSI { 3711}
(( segid "PROT" and resid 99 and name HN ))
(( segid "PROT" and resid 98 and name HB2 ))

```

```

3.100      2.400      2.400 peak 3711 weight 0 10000E+01 volume 0.26963E+01 ppm1      8.193 ppm2      3.033
ASSI { 3721}
(( segid "PROT" and resid 99 and name HN ))
( segid "PROT" and resid 99 and name HB*)
2.500      1.600      1.600 peak 3721 weight 0.10000E+01 volume 0.10441E+02 ppm1      8.191 ppm2      1.632
ASSI { 3731}
(( segid "PROT" and resid 64 and name HN ))
(( segid "PROT" and resid 64 and name HE1 ))
3.400      2.900      2.100 peak 3731 weight 0.10000E+01 volume 0.15156E+01 ppm1      8.019 ppm2      3.024
ASSI { 3761}
(( segid "PROT" and resid 22 and name HN ))
(( segid "PROT" and resid 22 and name HA ))
2.800      2.000      2.000 peak 3761 weight 0.10000E+01 volume 0.47526E+01 ppm1      8.854 ppm2      4.126
ASSI { 3771}
(( segid "PROT" and resid 22 and name HN ))
(( segid "PROT" and resid 22 and name HB1 ))
2.700      1.800      1.800 peak 3771 weight 0.10000E+01 volume 0.60546E+01 ppm1      8.854 ppm2      2.103
ASSI { 3781}
(( segid "PROT" and resid 22 and name HN ))
(( segid "PROT" and resid 21 and name HB ))
2.800      2.000      2.000 peak 3781 weight 0.10000E+01 volume 0.54991E+01 ppm1      8.856 ppm2      1.916
ASSI { 3791}
(( segid "PROT" and resid 22 and name HN ))
(( segid "PROT" and resid 22 and name HB2 ))
2.600      1.700      1.700 peak 3791 weight 0.10000E+01 volume 0.72128E+01 ppm1      8.853 ppm2      1.710
ASSI { 3801}
(( segid "PROT" and resid 22 and name HN ))
(( segid "PROT" and resid 19 and name HA ))
3.400      2.900      2.100 peak 3801 weight 0.10000E+01 volume 0.15388E+01 ppm1      8.849 ppm2      3.708
ASSI { 3821}
(( segid "PROT" and resid 22 and name HN ))
( segid "PROT" and resid 21 and name HG2*)
2.800      2.000      2.000 peak 3821 weight 0.10000E+01 volume 0.57390E+01 ppm1      8.853 ppm2      1.013
ASSI { 3831}
(( segid "PROT" and resid 25 and name HN ))
(( segid "PROT" and resid 23 and name HA ))
3.300      2.700      2.200 peak 3831 weight 0.10000E+01 volume 0.17967E+01 ppm1      8.565 ppm2      4.041
ASSI { 3841}
(( segid "PROT" and resid 25 and name HN ))
(( segid "PROT" and resid 24 and name HG1 ))
3.300      2.700      2.200 peak 3841 weight 0.10000E+01 volume 0.18150E+01 ppm1      8.571 ppm2      2.864
ASSI { 3861}
(( segid "PROT" and resid 25 and name HN ))
(( segid "PROT" and resid 28 and name HN ))
3.400      2.900      2.100 peak 3861 weight 0.10000E+01 volume 0.15678E+01 ppm1      8.564 ppm2      7.564
ASSI { 3871}
(( segid "PROT" and resid 25 and name HN ))
(( segid "PROT" and resid 22 and name HA ))
3.200      2.600      2.300 peak 3871 weight 0.10000E+01 volume 0.24333E+01 ppm1      8.563 ppm2      4.150
ASSI { 3881}
(( segid "PROT" and resid 25 and name HN ))
(( segid "PROT" and resid 25 and name HA ))
2.900      2.100      2.100 peak 3881 weight 0.10000E+01 volume 0.44045E+01 ppm1      8.563 ppm2      3.836
ASSI { 3891}
(( segid "PROT" and resid 25 and name HN ))
(( segid "PROT" and resid 24 and name HB2 ))
2.400      2.400      2.100 peak 3891 weight 0.10000E+01 volume 0.11850E+02 ppm1      8.565 ppm2      2.408
ASSI { 3901}
(( segid "PROT" and resid 25 and name HN ))
(( segid "PROT" and resid 25 and name HB ))
2.600      1.700      1.700 peak 3901 weight 0.10000E+01 volume 0.74683E+01 ppm1      8.565 ppm2      2.458
ASSI { 3911}
(( segid "PROT" and resid 25 and name HN ))
( segid "PROT" and resid 25 and name HG1*)
2.500      1.600      1.600 peak 3911 weight 0.10000E+01 volume 0.10519E+02 ppm1      8.564 ppm2      1.210
ASSI { 3921}
(( segid "PROT" and resid 25 and name HN ))
( segid "PROT" and resid 21 and name HG2*)
2.800      2.000      2.000 peak 3921 weight 0.10000E+01 volume 0.56705E+01 ppm1      8.565 ppm2      1.036
ASSI { 3941}
(( segid "PROT" and resid 76 and name HN ))
(( segid "PROT" and resid 74 and name HN ))
3.300      2.700      2.200 peak 3941 weight 0.10000E+01 volume 0.18542E+01 ppm1      8.021 ppm2      6.919
ASSI { 3951}
(( segid "PROT" and resid 101 and name HN ))
(( segid "PROT" and resid 98 and name HA ))
2.800      2.000      2.000 peak 3951 weight 0.10000E+01 volume 0.56914E+01 ppm1      8.017 ppm2      4.218
ASSI { 3961}
(( segid "PROT" and resid 76 and name HN ))
(( segid "PROT" and resid 75 and name HA ))
2.500      1.600      1.600 peak 3961 weight 0.10000E+01 volume 0.10452E+02 ppm1      8.020 ppm2      4.091
ASSI { 3971}
(( segid "PROT" and resid 101 and name HN ))
(( segid "PROT" and resid 99 and name HA ))
3.100      2.400      2.400 peak 3971 weight 0.10000E+01 volume 0.27135E+01 ppm1      8.020 ppm2      3.936
ASSI { 3981}
(( segid "PROT" and resid 76 and name HN ))
(( segid "PROT" and resid 74 and name HA ))
3.500      3.100      2.000 peak 3981 weight 0.10000E+01 volume 0.14645E+01 ppm1      8.019 ppm2      3.766

```

```

ASSI { 3991}
  (( segid "PROT" and resid 101 and name HN ))
  (( segid "PROT" and resid 100 and name HB1 ))
  2.800 2.000 2.000 peak 3991 weight 0.10000E+01 volume 0.46606E+01 ppm1 8.016 ppm2 2.920
ASSI { 4001}
  (( segid "PROT" and resid 101 and name HN ))
  (( segid "PROT" and resid 100 and name HA ))
  3.000 2.200 2.200 peak 4001 weight 0.10000E+01 volume 0.32888E+01 ppm1 8.015 ppm2 4.334
ASSI { 4011}
  (( segid "PROT" and resid 76 and name HN ))
  (( segid "PROT" and resid 75 and name HG1 ))
  2.900 2.100 2.100 peak 4011 weight 0.10000E+01 volume 0.42412E+01 ppm1 8.020 ppm2 2.320
ASSI { 4031}
  (( segid "PROT" and resid 101 and name HN ))
  (( segid "PROT" and resid 101 and name HA ))
  2.800 2.000 2.000 peak 4031 weight 0.10000E+01 volume 0.55917E+01 ppm1 8.014 ppm2 3.673
ASSI { 4041}
  (( segid "PROT" and resid 101 and name HN ))
  (( segid "PROT" and resid 100 and name HB2 ))
  3.000 2.200 2.200 peak 4041 weight 0.10000E+01 volume 0.35319E+01 ppm1 8.015 ppm2 2.818
ASSI { 4051}
  (( segid "PROT" and resid 101 and name HN ))
  (( segid "PROT" and resid 101 and name HG11))
  2.400 1.400 1.400 peak 4051 weight 0.10000E+01 volume 0.13903E+02 ppm1 8.014 ppm2 1.901
ASSI { 4061}
  (( segid "PROT" and resid 101 and name HN ))
  (( segid "PROT" and resid 101 and name HG12))
  2.900 2.100 2.100 peak 4061 weight 0.10000E+01 volume 0.44776E+01 ppm1 8.014 ppm2 1.223
ASSI { 4071}
  (( segid "PROT" and resid 101 and name HN ))
  (( segid "PROT" and resid 101 and name HD1%))
  2.600 1.700 1.700 peak 4071 weight 0.10000E+01 volume 0.77589E+01 ppm1 8.014 ppm2 0.990
ASSI { 4081}
  (( segid "PROT" and resid 96 and name HN ))
  (( segid "PROT" and resid 96 and name HD% ))
  3.200 2.600 2.300 peak 4081 weight 0.10000E+01 volume 0.23492E+01 ppm1 7.370 ppm2 7.132
ASSI { 4101}
  (( segid "PROT" and resid 96 and name HN ))
  (( segid "PROT" and resid 89 and name HB2 ))
  3.100 2.400 2.400 peak 4101 weight 0.10000E+01 volume 0.28581E+01 ppm1 7.368 ppm2 2.926
ASSI { 4111}
  (( segid "PROT" and resid 96 and name HN ))
  (( segid "PROT" and resid 96 and name HB2 ))
  2.800 2.000 2.000 peak 4111 weight 0.10000E+01 volume 0.54335E+01 ppm1 7.367 ppm2 2.566
ASSI { 4131}
  (( segid "PROT" and resid 96 and name HN ))
  (( segid "PROT" and resid 96 and name HA ))
  2.900 2.100 2.100 peak 4131 weight 0.10000E+01 volume 0.38508E+01 ppm1 7.361 ppm2 3.798
ASSI { 4141}
  (( segid "PROT" and resid 12 and name HN ))
  (( segid "PROT" and resid 12 and name HA ))
  2.500 1.600 1.600 peak 4141 weight 0.10000E+01 volume 0.10299E+02 ppm1 8.423 ppm2 4.706
ASSI { 4151}
  (( segid "PROT" and resid 12 and name HN ))
  (( segid "PROT" and resid 11 and name HD1 ))
  2.900 2.100 2.100 peak 4151 weight 0.10000E+01 volume 0.44553E+01 ppm1 8.423 ppm2 3.878
ASSI { 4161}
  (( segid "PROT" and resid 12 and name HN ))
  (( segid "PROT" and resid 15 and name HB2 ))
  3.600 3.200 1.900 peak 4161 weight 0.10000E+01 volume 0.12071E+01 ppm1 8.424 ppm2 3.067
ASSI { 4171}
  (( segid "PROT" and resid 12 and name HN ))
  (( segid "PROT" and resid 12 and name HB2 ))
  2.500 1.600 1.600 peak 4171 weight 0.10000E+01 volume 0.10156E+02 ppm1 8.422 ppm2 2.762
ASSI { 4181}
  (( segid "PROT" and resid 12 and name HN ))
  (( segid "PROT" and resid 11 and name HB1 ))
  3.300 2.700 2.200 peak 4181 weight 0.10000E+01 volume 0.18905E+01 ppm1 8.423 ppm2 2.358
ASSI { 4191}
  (( segid "PROT" and resid 12 and name HN ))
  (( segid "PROT" and resid 13 and name HB1 ))
  3.300 2.700 2.200 peak 4191 weight 0.10000E+01 volume 0.19426E+01 ppm1 8.422 ppm2 2.160
ASSI { 4201}
  (( segid "PROT" and resid 12 and name HN ))
  (( segid "PROT" and resid 11 and name HB2 ))
  2.900 2.100 2.100 peak 4201 weight 0.10000E+01 volume 0.38127E+01 ppm1 8.424 ppm2 2.084
ASSI { 4211}
  (( segid "PROT" and resid 12 and name HN ))
  (( segid "PROT" and resid 13 and name HN ))
  2.600 1.700 1.700 peak 4211 weight 0.10000E+01 volume 0.86085E+01 ppm1 8.421 ppm2 8.184
ASSI { 4221}
  (( segid "PROT" and resid 12 and name HN ))
  (( segid "PROT" and resid 10 and name HA ))
  3.600 3.200 1.900 peak 4221 weight 0.10000E+01 volume 0.11464E+01 ppm1 8.420 ppm2 4.904
ASSI { 4231}
  (( segid "PROT" and resid 12 and name HN ))
  (( segid "PROT" and resid 11 and name HA ))
  2.800 2.000 2.000 peak 4231 weight 0.10000E+01 volume 0.54533E+01 ppm1 8.421 ppm2 4.353
ASSI { 4251}

```

```

(( segid "PROT" and resid 76 and name HN ))
(( segid "PROT" and resid 75 and name HB2 ))
3.400 2.900 2.100 peak 4251 weight 0.10000E+01 volume 0.17162E+01 ppm1 8.022 ppm2 2.617
ASSI { 4261}
(( segid "PROT" and resid 76 and name HN ))
(( segid "PROT" and resid 75 and name HG2 ))
2.800 2.000 2.000 peak 4261 weight 0.10000E+01 volume 0.53106E+01 ppm1 8.020 ppm2 2.216
ASSI { 4271}
(( segid "PROT" and resid 76 and name HN ))
(( segid "PROT" and resid 76 and name HB% ))
2.200 1.200 1.200 peak 4271 weight 0.10000E+01 volume 0.22283E+02 ppm1 8.021 ppm2 1.511
ASSI { 4291}
(( segid "PROT" and resid 78 and name HN ))
(( segid "PROT" and resid 77 and name HA ))
2.700 1.800 1.800 peak 4291 weight 0.10000E+01 volume 0.65577E+01 ppm1 7.380 ppm2 4.367
ASSI { 4301}
(( segid "PROT" and resid 78 and name HN ))
(( segid "PROT" and resid 75 and name HA ))
2.900 2.100 2.100 peak 4301 weight 0.10000E+01 volume 0.39670E+01 ppm1 7.381 ppm2 4.089
ASSI { 4311}
(( segid "PROT" and resid 78 and name HN ))
(( segid "PROT" and resid 78 and name HA ))
2.800 2.000 2.000 peak 4311 weight 0.10000E+01 volume 0.53868E+01 ppm1 7.380 ppm2 3.389
ASSI { 4321}
(( segid "PROT" and resid 78 and name HN ))
(( segid "PROT" and resid 80 and name HB1 ))
3.300 2.700 2.200 peak 4321 weight 0.10000E+01 volume 0.21033E+01 ppm1 7.381 ppm2 1.980
ASSI { 4361}
(( segid "PROT" and resid 96 and name HN ))
(( segid "PROT" and resid 94 and name HA ))
3.200 2.600 2.300 peak 4361 weight 0.10000E+01 volume 0.24482E+01 ppm1 7.375 ppm2 4.225
ASSI { 4371}
(( segid "PROT" and resid 78 and name HN ))
(( segid "PROT" and resid 77 and name HB1 ))
2.500 1.600 1.600 peak 4371 weight 0.10000E+01 volume 0.10999E+02 ppm1 7.379 ppm2 2.729
ASSI { 4381}
(( segid "PROT" and resid 77 and name HN ))
(( segid "PROT" and resid 76 and name HB% ))
2.500 1.600 1.600 peak 4381 weight 0.10000E+01 volume 0.10974E+02 ppm1 7.379 ppm2 1.510
ASSI { 4401}
(( segid "PROT" and resid 89 and name HD22))
(( segid "PROT" and resid 89 and name HD21))
3.000 2.200 2.200 peak 4401 weight 0.10000E+01 volume 0.32494E+01 ppm1 7.821 ppm2 8.354
ASSI { 4411}
(( segid "PROT" and resid 78 and name HN ))
(( segid "PROT" and resid 79 and name HN ))
2.600 1.700 1.700 peak 4411 weight 0.10000E+01 volume 0.77884E+01 ppm1 7.385 ppm2 8.099
ASSI { 4421}
(( segid "PROT" and resid 78 and name HN ))
(( segid "PROT" and resid 79 and name HB1 ))
3.300 2.700 2.200 peak 4421 weight 0.10000E+01 volume 0.19297E+01 ppm1 7.385 ppm2 2.189
ASSI { 4431}
(( segid "PROT" and resid 78 and name HN ))
(( segid "PROT" and resid 59 and name HB% ))
2.700 1.800 1.800 peak 4431 weight 0.10000E+01 volume 0.62776E+01 ppm1 7.384 ppm2 1.280
ASSI { 4441}
(( segid "PROT" and resid 78 and name HN ))
(( segid "PROT" and resid 78 and name HB1 ))
2.600 1.700 1.700 peak 4441 weight 0.10000E+01 volume 0.76075E+01 ppm1 7.385 ppm2 0.719
ASSI { 4451}
(( segid "PROT" and resid 78 and name HN ))
(( segid "PROT" and resid 78 and name HB2 ))
2.600 1.700 1.700 peak 4451 weight 0.10000E+01 volume 0.90536E+01 ppm1 7.384 ppm2 0.446
ASSI { 4461}
(( segid "PROT" and resid 78 and name HN ))
(( segid "PROT" and resid 78 and name HD2% ))
3.300 2.700 2.200 peak 4461 weight 0.10000E+01 volume 0.20077E+01 ppm1 7.386 ppm2 0.169
ASSI { 4471}
(( segid "PROT" and resid 78 and name HN ))
(( segid "PROT" and resid 78 and name HD1% ))
3.200 2.600 2.300 peak 4471 weight 0.10000E+01 volume 0.22843E+01 ppm1 7.387 ppm2 0.070
ASSI { 4491}
(( segid "PROT" and resid 54 and name HN ))
(( segid "PROT" and resid 55 and name HN ))
2.900 2.100 2.100 peak 4491 weight 0.10000E+01 volume 0.44496E+01 ppm1 8.520 ppm2 7.416
ASSI { 4501}
(( segid "PROT" and resid 54 and name HN ))
(( segid "PROT" and resid 54 and name HA ))
3.200 2.600 2.300 peak 4501 weight 0.10000E+01 volume 0.24899E+01 ppm1 8.520 ppm2 4.962
ASSI { 4521}
(( segid "PROT" and resid 54 and name HN ))
(( segid "PROT" and resid 53 and name HB1 ))
3.000 2.200 2.200 peak 4521 weight 0.10000E+01 volume 0.31395E+01 ppm1 8.520 ppm2 2.246
ASSI { 4531}
(( segid "PROT" and resid 54 and name HN ))
(( segid "PROT" and resid 54 and name HG2 ))
3.300 2.700 2.200 peak 4531 weight 0.10000E+01 volume 0.17850E+01 ppm1 8.520 ppm2 1.915
ASSI { 4541}
(( segid "PROT" and resid 54 and name HN ))

```

```

(( segid "PROT" and resid 54 and name HB2 ))
3.400 2.900 2.100 peak 4541 weight 0.10000E+01 volume 0.17029E+01 ppm1 8.526 ppm2 1.348
ASSI { 4551}
(( segid "PROT" and resid 54 and name HN ))
(( segid "PROT" and resid 50 and name HG2% ))
3.300 2.700 2.200 peak 4551 weight 0.10000E+01 volume 0.17768E+01 ppm1 8.520 ppm2 0.397
ASSI { 4561}
(( segid "PROT" and resid 54 and name HN ))
(( segid "PROT" and resid 53 and name HA ))
2.600 1.700 1.700 peak 4561 weight 0.10000E+01 volume 0.77293E+01 ppm1 8.518 ppm2 4.099
ASSI { 4571}
(( segid "PROT" and resid 54 and name HN ))
(( segid "PROT" and resid 80 and name HB2 ))
3.300 2.700 2.200 peak 4571 weight 0.10000E+01 volume 0.19268E+01 ppm1 8.520 ppm2 1.983
ASSI { 4581}
(( segid "PROT" and resid 30 and name HN ))
(( segid "PROT" and resid 29 and name HN ))
3.000 2.200 2.200 peak 4581 weight 0.10000E+01 volume 0.31596E+01 ppm1 11.696 ppm2 8.578
ASSI { 4591}
(( segid "PROT" and resid 30 and name HN ))
(( segid "PROT" and resid 31 and name HN ))
2.700 1.800 1.800 peak 4591 weight 0.10000E+01 volume 0.65999E+01 ppm1 11.698 ppm2 7.913
ASSI { 4601}
(( segid "PROT" and resid 30 and name HN ))
(( segid "PROT" and resid 30 and name HA ))
3.000 2.200 2.200 peak 4601 weight 0.10000E+01 volume 0.34965E+01 ppm1 11.695 ppm2 4.829
ASSI { 4611}
(( segid "PROT" and resid 30 and name HN ))
(( segid "PROT" and resid 30 and name HB1 ))
3.100 2.400 2.400 peak 4611 weight 0.10000E+01 volume 0.28201E+01 ppm1 11.695 ppm2 4.332
ASSI { 4621}
(( segid "PROT" and resid 30 and name HN ))
(( segid "PROT" and resid 29 and name HA ))
3.200 2.600 2.300 peak 4621 weight 0.10000E+01 volume 0.22951E+01 ppm1 11.698 ppm2 4.226
ASSI { 4631}
(( segid "PROT" and resid 30 and name HN ))
(( segid "PROT" and resid 30 and name HB2 ))
2.900 2.100 2.100 peak 4631 weight 0.10000E+01 volume 0.40640E+01 ppm1 11.695 ppm2 3.957
ASSI { 4641}
(( segid "PROT" and resid 30 and name HN ))
(( segid "PROT" and resid 29 and name HB1 ))
3.100 2.400 2.400 peak 4641 weight 0.10000E+01 volume 0.30464E+01 ppm1 11.694 ppm2 2.126
ASSI { 4651}
(( segid "PROT" and resid 30 and name HN ))
(( segid "PROT" and resid 31 and name HB% ))
3.500 3.100 2.000 peak 4651 weight 0.10000E+01 volume 0.12947E+01 ppm1 11.693 ppm2 1.735
ASSI { 4661}
(( segid "PROT" and resid 30 and name HN ))
(( segid "PROT" and resid 101 and name HG2% ))
3.600 3.200 1.900 peak 4661 weight 0.10000E+01 volume 0.11385E+01 ppm1 11.694 ppm2 1.011
ASSI { 4681}
(( segid "PROT" and resid 30 and name HN ))
(( segid "PROT" and resid 28 and name HN ))
3.400 2.900 2.100 peak 4681 weight 0.10000E+01 volume 0.16627E+01 ppm1 11.691 ppm2 7.563
ASSI { 4701}
(( segid "PROT" and resid 15 and name HN ))
(( segid "PROT" and resid 14 and name HN ))
2.400 1.400 1.400 peak 4701 weight 0.10000E+01 volume 0.11587E+02 ppm1 7.994 ppm2 8.197
ASSI { 4711}
(( segid "PROT" and resid 15 and name HN ))
(( segid "PROT" and resid 15 and name HD% ))
3.400 2.900 2.100 peak 4711 weight 0.10000E+01 volume 0.16091E+01 ppm1 7.996 ppm2 7.070
ASSI { 4721}
(( segid "PROT" and resid 15 and name HN ))
(( segid "PROT" and resid 15 and name HA ))
2.600 1.700 1.700 peak 4721 weight 0.10000E+01 volume 0.74337E+01 ppm1 7.995 ppm2 4.026
ASSI { 4741}
(( segid "PROT" and resid 15 and name HN ))
(( segid "PROT" and resid 15 and name HB1 ))
2.600 1.700 1.700 peak 4741 weight 0.10000E+01 volume 0.86825E+01 ppm1 7.994 ppm2 3.218
ASSI { 4751}
(( segid "PROT" and resid 15 and name HN ))
(( segid "PROT" and resid 15 and name HB2 ))
2.600 1.700 1.700 peak 4751 weight 0.10000E+01 volume 0.82436E+01 ppm1 7.993 ppm2 3.047
ASSI { 4761}
(( segid "PROT" and resid 15 and name HN ))
(( segid "PROT" and resid 14 and name HB1 ))
2.900 2.100 2.100 peak 4761 weight 0.10000E+01 volume 0.43406E+01 ppm1 7.994 ppm2 1.858
ASSI { 4771}
(( segid "PROT" and resid 15 and name HN ))
(( segid "PROT" and resid 14 and name HB2 ))
3.000 2.200 2.200 peak 4771 weight 0.10000E+01 volume 0.36582E+01 ppm1 7.997 ppm2 1.572
ASSI { 4781}
(( segid "PROT" and resid 15 and name HN ))
(( segid "PROT" and resid 14 and name HG ))
3.300 2.700 2.200 peak 4781 weight 0.10000E+01 volume 0.20741E+01 ppm1 7.996 ppm2 1.467
ASSI { 4791}
(( segid "PROT" and resid 15 and name HN ))
(( segid "PROT" and resid 14 and name HD2% ))

```

```

3.100      2.400      2.400 peak 4791 weight 0.10000E+01 volume 0.29619E+01 ppm1 7.992 ppm2 0.817
ASSI { 4801}
(( segid "PROT" and resid 15 and name HN ))
(( segid "PROT" and resid 12 and name HA ))
3.000      2.200      2.200 peak 4801 weight 0.10000E+01 volume 0.37120E+01 ppm1 7.990 ppm2 4.731
ASSI { 4821}
(( segid "PROT" and resid 55 and name HN ))
(( segid "PROT" and resid 54 and name HA ))
2.500      1.600      1.600 peak 4821 weight 0.10000E+01 volume 0.10125E+02 ppm1 7.380 ppm2 4.956
ASSI { 4831}
(( segid "PROT" and resid 55 and name HN ))
(( segid "PROT" and resid 55 and name HA ))
2.600      1.700      1.700 peak 4831 weight 0.10000E+01 volume 0.84076E+01 ppm1 7.383 ppm2 4.742
ASSI { 4841}
(( segid "PROT" and resid 55 and name HN ))
(( segid "PROT" and resid 54 and name HG1 ))
3.100      2.400      2.400 peak 4841 weight 0.10000E+01 volume 0.27028E+01 ppm1 7.382 ppm2 2.706
ASSI { 4851}
(( segid "PROT" and resid 55 and name HN ))
(( segid "PROT" and resid 59 and name HG2 ))
3.600      3.200      1.900 peak 4851 weight 0.10000E+01 volume 0.12119E+01 ppm1 7.386 ppm2 2.546
ASSI { 4861}
(( segid "PROT" and resid 55 and name HN ))
(( segid "PROT" and resid 54 and name HB2 ))
3.500      3.100      2.000 peak 4861 weight 0.10000E+01 volume 0.14758E+01 ppm1 7.385 ppm2 1.352
ASSI { 4871}
(( segid "PROT" and resid 55 and name HN ))
(( segid "PROT" and resid 58 and name HG2% ))
3.200      2.600      2.300 peak 4871 weight 0.10000E+01 volume 0.24734E+01 ppm1 7.381 ppm2 1.072
ASSI { 4881}
(( segid "PROT" and resid 55 and name HN ))
(( segid "PROT" and resid 81 and name HG1% ))
3.100      2.400      2.400 peak 4881 weight 0.10000E+01 volume 0.28394E+01 ppm1 7.383 ppm2 0.476
ASSI { 4891}
(( segid "PROT" and resid 55 and name HN ))
(( segid "PROT" and resid 55 and name HB1 ))
3.200      2.600      2.300 peak 4891 weight 0.10000E+01 volume 0.22382E+01 ppm1 7.378 ppm2 2.376
ASSI { 4901}
(( segid "PROT" and resid 24 and name HN ))
(( segid "PROT" and resid 27 and name HN ))
3.500      3.100      2.000 peak 4901 weight 0.10000E+01 volume 0.12574E+01 ppm1 8.045 ppm2 7.569
ASSI { 4921}
(( segid "PROT" and resid 74 and name HN ))
(( segid "PROT" and resid 18 and name HD2% ))
3.500      3.100      2.000 peak 4921 weight 0.10000E+01 volume 0.12668E+01 ppm1 6.927 ppm2 -0.183
ASSI { 4931}
(( segid "PROT" and resid 74 and name HN ))
(( segid "PROT" and resid 73 and name HD2% ))
3.500      3.100      2.000 peak 4931 weight 0.10000E+01 volume 0.14113E+01 ppm1 6.917 ppm2 0.943
ASSI { 4941}
(( segid "PROT" and resid 19 and name HN ))
(( segid "PROT" and resid 18 and name HD2% ))
3.500      3.100      2.000 peak 4941 weight 0.10000E+01 volume 0.12909E+01 ppm1 8.569 ppm2 -0.181
ASSI { 4951}
(( segid "PROT" and resid 24 and name HN ))
(( segid "PROT" and resid 25 and name HG1% ))
3.500      3.100      2.000 peak 4951 weight 0.10000E+01 volume 0.14575E+01 ppm1 8.048 ppm2 1.208
ASSI { 4961}
(( segid "PROT" and resid 24 and name HN ))
(( segid "PROT" and resid 25 and name HN ))
2.300      1.300      1.300 peak 4961 weight 0.10000E+01 volume 0.15441E+02 ppm1 8.046 ppm2 8.568
ASSI { 4971}
(( segid "PROT" and resid 24 and name HN ))
(( segid "PROT" and resid 24 and name HE21 ))
3.600      3.200      1.900 peak 4971 weight 0.10000E+01 volume 0.12268E+01 ppm1 8.044 ppm2 7.031
ASSI { 4981}
(( segid "PROT" and resid 24 and name HN ))
(( segid "PROT" and resid 24 and name HA ))
2.800      2.000      2.000 peak 4981 weight 0.10000E+01 volume 0.51016E+01 ppm1 8.045 ppm2 4.194
ASSI { 5001}
(( segid "PROT" and resid 24 and name HN ))
(( segid "PROT" and resid 21 and name HA ))
3.200      2.600      2.300 peak 5001 weight 0.10000E+01 volume 0.23114E+01 ppm1 8.046 ppm2 3.782
ASSI { 5011}
(( segid "PROT" and resid 24 and name HN ))
(( segid "PROT" and resid 24 and name HG1 ))
2.600      1.700      1.700 peak 5011 weight 0.10000E+01 volume 0.77445E+01 ppm1 8.045 ppm2 2.866
ASSI { 5021}
(( segid "PROT" and resid 24 and name HN ))
(( segid "PROT" and resid 24 and name HB1 ))
2.400      1.400      1.400 peak 5021 weight 0.10000E+01 volume 0.13011E+02 ppm1 8.045 ppm2 2.480
ASSI { 5031}
(( segid "PROT" and resid 24 and name HN ))
(( segid "PROT" and resid 24 and name HB2 ))
2.600      1.700      1.700 peak 5031 weight 0.10000E+01 volume 0.77725E+01 ppm1 8.045 ppm2 2.386
ASSI { 5041}
(( segid "PROT" and resid 24 and name HN ))
(( segid "PROT" and resid 23 and name HB2 ))
2.900      2.100      2.100 peak 5041 weight 0.10000E+01 volume 0.45542E+01 ppm1 8.045 ppm2 2.241

```



```

ASSI { 5051}
(( segid "PROT" and resid 24 and name HN ))
(( segid "PROT" and resid 22 and name HB1 ))
3.500 3.100 2.000 peak 5051 weight 0.10000E+01 volume 0.12517E+01 ppm1 8.044 ppm2 2.103
ASSI { 5061}
(( segid "PROT" and resid 24 and name HN ))
(( segid "PROT" and resid 25 and name HG2% ))
3.500 3.100 2.000 peak 5061 weight 0.10000E+01 volume 0.14572E+01 ppm1 8.043 ppm2 1.018
ASSI { 5081}
(( segid "PROT" and resid 73 and name HN ))
(( segid "PROT" and resid 75 and name HN ))
3.500 3.100 2.000 peak 5081 weight 0.10000E+01 volume 0.12647E+01 ppm1 7.444 ppm2 8.505
ASSI { 5101}
(( segid "PROT" and resid 73 and name HN ))
(( segid "PROT" and resid 74 and name HN ))
2.600 1.700 1.700 peak 5101 weight 0.10000E+01 volume 0.80031E+01 ppm1 7.442 ppm2 6.928
ASSI { 5111}
(( segid "PROT" and resid 73 and name HN ))
(( segid "PROT" and resid 70 and name HB1 ))
2.700 1.800 1.800 peak 5111 weight 0.10000E+01 volume 0.70510E+01 ppm1 7.440 ppm2 4.231
ASSI { 5121}
(( segid "PROT" and resid 73 and name HN ))
(( segid "PROT" and resid 73 and name HD2% ))
3.000 2.200 2.200 peak 5121 weight 0.10000E+01 volume 0.34221E+01 ppm1 7.444 ppm2 0.928
ASSI { 5131}
(( segid "PROT" and resid 73 and name HN ))
(( segid "PROT" and resid 73 and name HG ))
2.500 1.600 1.600 peak 5131 weight 0.10000E+01 volume 0.99511E+01 ppm1 7.434 ppm2 1.777
ASSI { 5141}
(( segid "PROT" and resid 80 and name HN ))
(( segid "PROT" and resid 80 and name HB2 ))
2.400 1.400 1.400 peak 5141 weight 0.10000E+01 volume 0.14158E+02 ppm1 7.422 ppm2 1.988
ASSI { 5161}
(( segid "PROT" and resid 80 and name HN ))
(( segid "PROT" and resid 76 and name HB% ))
3.200 2.600 2.300 peak 5161 weight 0.10000E+01 volume 0.21895E+01 ppm1 7.427 ppm2 1.508
ASSI { 5181}
(( segid "PROT" and resid 80 and name HN ))
(( segid "PROT" and resid 81 and name HN ))
2.600 1.700 1.700 peak 5181 weight 0.10000E+01 volume 0.75351E+01 ppm1 7.416 ppm2 7.031
ASSI { 5191}
(( segid "PROT" and resid 80 and name HN ))
(( segid "PROT" and resid 80 and name HA ))
2.600 1.700 1.700 peak 5191 weight 0.10000E+01 volume 0.74789E+01 ppm1 7.417 ppm2 4.072
ASSI { 5201}
(( segid "PROT" and resid 80 and name HN ))
(( segid "PROT" and resid 79 and name HA ))
3.200 2.600 2.300 peak 5201 weight 0.10000E+01 volume 0.22928E+01 ppm1 7.419 ppm2 3.815
ASSI { 5211}
(( segid "PROT" and resid 80 and name HN ))
(( segid "PROT" and resid 78 and name HA ))
3.500 3.100 2.000 peak 5211 weight 0.10000E+01 volume 0.12621E+01 ppm1 7.416 ppm2 3.386
ASSI { 5221}
(( segid "PROT" and resid 80 and name HN ))
(( segid "PROT" and resid 79 and name HB1 ))
2.900 2.100 2.100 peak 5221 weight 0.10000E+01 volume 0.39082E+01 ppm1 7.416 ppm2 2.187
ASSI { 5231}
(( segid "PROT" and resid 80 and name HN ))
(( segid "PROT" and resid 79 and name HG1 ))
3.300 2.700 2.200 peak 5231 weight 0.10000E+01 volume 0.18927E+01 ppm1 7.413 ppm2 2.441
ASSI { 5251}
(( segid "PROT" and resid 74 and name HN ))
(( segid "PROT" and resid 70 and name HB1 ))
3.300 2.700 2.200 peak 5251 weight 0.10000E+01 volume 0.20701E+01 ppm1 6.926 ppm2 4.229
ASSI { 5261}
(( segid "PROT" and resid 74 and name HN ))
(( segid "PROT" and resid 75 and name HN ))
2.700 1.800 1.800 peak 5261 weight 0.10000E+01 volume 0.70119E+01 ppm1 6.922 ppm2 8.499
ASSI { 5281}
(( segid "PROT" and resid 24 and name HE22 ))
(( segid "PROT" and resid 109 and name HA ))
3.100 2.400 2.400 peak 5281 weight 0.10000E+01 volume 0.27313E+01 ppm1 6.921 ppm2 4.037
ASSI { 5291}
(( segid "PROT" and resid 74 and name HN ))
(( segid "PROT" and resid 74 and name HA ))
3.000 2.200 2.200 peak 5291 weight 0.10000E+01 volume 0.37588E+01 ppm1 6.920 ppm2 3.782
ASSI { 5301}
(( segid "PROT" and resid 74 and name HN ))
(( segid "PROT" and resid 74 and name HB1 ))
2.700 1.800 1.800 peak 5301 weight 0.10000E+01 volume 0.68724E+01 ppm1 6.922 ppm2 2.958
ASSI { 5311}
(( segid "PROT" and resid 74 and name HN ))
(( segid "PROT" and resid 74 and name HB2 ))
2.800 2.000 2.000 peak 5311 weight 0.10000E+01 volume 0.49112E+01 ppm1 6.923 ppm2 2.394
ASSI { 5321}
(( segid "PROT" and resid 74 and name HN ))
(( segid "PROT" and resid 73 and name HB1 ))
3.100 2.400 2.400 peak 5321 weight 0.10000E+01 volume 0.30104E+01 ppm1 6.924 ppm2 1.999
ASSI { 5331}

```

```

(( segid "PROT" and resid 74 and name HN ))
(( segid "PROT" and resid 73 and name HB2 ))
3.000 2.200 2.200 peak 5331 weight 0.10000E+01 volume 0.34844E+01 ppm1 6.921 ppm2 1.893
ASSI { 5341}
(( segid "PROT" and resid 74 and name HN ))
(( segid "PROT" and resid 73 and name HG ))
3.400 2.900 2.100 peak 5341 weight 0.10000E+01 volume 0.17239E+01 ppm1 6.921 ppm2 1.778
ASSI { 5351}
(( segid "PROT" and resid 74 and name HN ))
(( segid "PROT" and resid 18 and name HD1% ))
3.500 3.100 2.000 peak 5351 weight 0.10000E+01 volume 0.12974E+01 ppm1 6.921 ppm2 0.480
ASSI { 5361}
(( segid "PROT" and resid 24 and name HE22 ))
(( segid "PROT" and resid 24 and name HN ))
3.600 3.200 1.900 peak 5361 weight 0.10000E+01 volume 0.11576E+01 ppm1 6.910 ppm2 8.026
ASSI { 5381}
(( segid "PROT" and resid 19 and name HN ))
(( segid "PROT" and resid 17 and name HG2% ))
3.400 2.900 2.100 peak 5381 weight 0.10000E+01 volume 0.15290E+01 ppm1 8.578 ppm2 1.151
ASSI { 5391}
(( segid "PROT" and resid 19 and name HN ))
(( segid "PROT" and resid 18 and name HD1% ))
3.500 3.100 2.000 peak 5391 weight 0.10000E+01 volume 0.14602E+01 ppm1 8.576 ppm2 0.482
ASSI { 5421}
(( segid "PROT" and resid 19 and name HN ))
(( segid "PROT" and resid 15 and name HA ))
3.200 2.600 2.300 peak 5421 weight 0.10000E+01 volume 0.24616E+01 ppm1 8.574 ppm2 4.029
ASSI { 5431}
(( segid "PROT" and resid 19 and name HN ))
(( segid "PROT" and resid 17 and name HA ))
3.000 2.200 2.200 peak 5431 weight 0.10000E+01 volume 0.32388E+01 ppm1 8.573 ppm2 3.928
ASSI { 5441}
(( segid "PROT" and resid 19 and name HN ))
(( segid "PROT" and resid 19 and name HA ))
2.800 2.000 2.000 peak 5441 weight 0.10000E+01 volume 0.54958E+01 ppm1 8.574 ppm2 3.693
ASSI { 5451}
(( segid "PROT" and resid 19 and name HN ))
(( segid "PROT" and resid 18 and name HA ))
3.300 2.700 2.200 peak 5451 weight 0.10000E+01 volume 0.18487E+01 ppm1 8.571 ppm2 3.290
ASSI { 5461}
(( segid "PROT" and resid 19 and name HN ))
(( segid "PROT" and resid 19 and name HB1 ))
2.600 1.700 1.700 peak 5461 weight 0.10000E+01 volume 0.87577E+01 ppm1 8.574 ppm2 1.703
ASSI { 5471}
(( segid "PROT" and resid 19 and name HN ))
(( segid "PROT" and resid 18 and name HB1 ))
2.900 2.100 2.100 peak 5471 weight 0.10000E+01 volume 0.39883E+01 ppm1 8.575 ppm2 1.531
ASSI { 5481}
(( segid "PROT" and resid 19 and name HN ))
(( segid "PROT" and resid 19 and name HB2 ))
2.600 1.700 1.700 peak 5481 weight 0.10000E+01 volume 0.78056E+01 ppm1 8.574 ppm2 1.378
ASSI { 5491}
(( segid "PROT" and resid 19 and name HN ))
(( segid "PROT" and resid 19 and name HG1 ))
2.800 2.000 2.000 peak 5491 weight 0.10000E+01 volume 0.49710E+01 ppm1 8.575 ppm2 1.282
ASSI { 5501}
(( segid "PROT" and resid 19 and name HN ))
(( segid "PROT" and resid 63 and name HD2% ))
3.100 2.400 2.400 peak 5501 weight 0.10000E+01 volume 0.27977E+01 ppm1 8.573 ppm2 1.044
ASSI { 5511}
(( segid "PROT" and resid 19 and name HN ))
(( segid "PROT" and resid 63 and name HD1% ))
3.000 2.200 2.200 peak 5511 weight 0.10000E+01 volume 0.32125E+01 ppm1 8.573 ppm2 0.891
ASSI { 5521}
(( segid "PROT" and resid 19 and name HN ))
(( segid "PROT" and resid 18 and name HB2 ))
3.200 2.600 2.300 peak 5521 weight 0.10000E+01 volume 0.25168E+01 ppm1 8.574 ppm2 0.321
ASSI { 5531}
(( segid "PROT" and resid 19 and name HN ))
(( segid "PROT" and resid 17 and name HB ))
3.400 2.900 2.100 peak 5531 weight 0.10000E+01 volume 0.15384E+01 ppm1 8.566 ppm2 4.264
ASSI { 5541}
(( segid "PROT" and resid 80 and name HN ))
(( segid "PROT" and resid 77 and name HA ))
3.300 2.700 2.200 peak 5541 weight 0.10000E+01 volume 0.19122E+01 ppm1 7.416 ppm2 4.370
ASSI { 5551}
(( segid "PROT" and resid 42 and name HN ))
(( segid "PROT" and resid 39 and name HB2 ))
3.000 2.200 2.200 peak 5551 weight 0.10000E+01 volume 0.31705E+01 ppm1 7.210 ppm2 1.919
ASSI { 5561}
(( segid "PROT" and resid 42 and name HN ))
(( segid "PROT" and resid 42 and name HA ))
2.800 2.000 2.000 peak 5561 weight 0.10000E+01 volume 0.47858E+01 ppm1 7.204 ppm2 4.477
ASSI { 5571}
(( segid "PROT" and resid 42 and name HN ))
(( segid "PROT" and resid 41 and name HB ))
3.400 2.900 2.100 peak 5571 weight 0.10000E+01 volume 0.16358E+01 ppm1 7.202 ppm2 4.338
ASSI { 5581}
(( segid "PROT" and resid 42 and name HN ))

```

```

(( segid "PROT" and resid 41 and name HA ))
3.100 2.400 2.400 peak 5581 weight 0.10000E+01 volume 0.25691E+01 ppm1 7.204 ppm2 4.074
ASSI { 5591}
(( segid "PROT" and resid 42 and name HN ))
(( segid "PROT" and resid 42 and name HG2 ))
3.000 2.200 2.200 peak 5591 weight 0.10000E+01 volume 0.35712E+01 ppm1 7.204 ppm2 2.268
ASSI { 5601}
(( segid "PROT" and resid 42 and name HN ))
(( segid "PROT" and resid 42 and name HB1 ))
2.900 2.100 2.100 peak 5601 weight 0.10000E+01 volume 0.42597E+01 ppm1 7.207 ppm2 2.194
ASSI { 5611}
(( segid "PROT" and resid 42 and name HN ))
(( segid "PROT" and resid 42 and name HB2 ))
2.800 2.000 2.000 peak 5611 weight 0.10000E+01 volume 0.53742E+01 ppm1 7.207 ppm2 2.046
ASSI { 5621}
(( segid "PROT" and resid 42 and name HN ))
(( segid "PROT" and resid 42 and name HG1 ))
3.200 2.600 2.300 peak 5621 weight 0.10000E+01 volume 0.24540E+01 ppm1 7.206 ppm2 2.334
ASSI { 5631}
(( segid "PROT" and resid 42 and name HN ))
(( segid "PROT" and resid 39 and name HD2 ))
3.100 2.400 2.400 peak 5631 weight 0.10000E+01 volume 0.30124E+01 ppm1 7.204 ppm2 1.650
ASSI { 5641}
(( segid "PROT" and resid 42 and name HN ))
(( segid "PROT" and resid 39 and name HG2 ))
3.500 3.100 2.000 peak 5641 weight 0.10000E+01 volume 0.12606E+01 ppm1 7.205 ppm2 1.455
ASSI { 5651}
(( segid "PROT" and resid 42 and name HN ))
(( segid "PROT" and resid 38 and name HG2% ))
3.600 3.200 1.900 peak 5651 weight 0.10000E+01 volume 0.11209E+01 ppm1 7.202 ppm2 -0.032
ASSI { 5661}
(( segid "PROT" and resid 42 and name HN ))
(( segid "PROT" and resid 43 and name HB% ))
3.500 3.100 2.000 peak 5661 weight 0.10000E+01 volume 0.14702E+01 ppm1 7.203 ppm2 0.963
ASSI { 5671}
(( segid "PROT" and resid 107 and name HN ))
(( segid "PROT" and resid 107 and name HD% ))
3.400 2.900 2.100 peak 5671 weight 0.10000E+01 volume 0.17606E+01 ppm1 8.406 ppm2 7.197
ASSI { 5691}
(( segid "PROT" and resid 107 and name HN ))
(( segid "PROT" and resid 110 and name HN ))
3.500 3.100 2.000 peak 5691 weight 0.10000E+01 volume 0.13382E+01 ppm1 8.401 ppm2 8.129
ASSI { 5731}
(( segid "PROT" and resid 107 and name HN ))
(( segid "PROT" and resid 106 and name HD% ))
3.500 3.100 2.000 peak 5731 weight 0.10000E+01 volume 0.14164E+01 ppm1 8.405 ppm2 6.913
ASSI { 5741}
(( segid "PROT" and resid 107 and name HN ))
(( segid "PROT" and resid 106 and name HA ))
3.000 2.200 2.200 peak 5741 weight 0.10000E+01 volume 0.33201E+01 ppm1 8.401 ppm2 3.973
ASSI { 5751}
(( segid "PROT" and resid 107 and name HN ))
(( segid "PROT" and resid 107 and name HA ))
2.700 1.800 1.800 peak 5751 weight 0.10000E+01 volume 0.58816E+01 ppm1 8.402 ppm2 3.841
ASSI { 5761}
(( segid "PROT" and resid 107 and name HN ))
(( segid "PROT" and resid 106 and name HB1 ))
2.900 2.100 2.100 peak 5761 weight 0.10000E+01 volume 0.42118E+01 ppm1 8.403 ppm2 3.311
ASSI { 5771}
(( segid "PROT" and resid 107 and name HN ))
(( segid "PROT" and resid 107 and name HB1 ))
2.300 1.300 1.300 peak 5771 weight 0.10000E+01 volume 0.18413E+02 ppm1 8.402 ppm2 3.073
ASSI { 5781}
(( segid "PROT" and resid 87 and name HN ))
(( segid "PROT" and resid 50 and name HD1% ))
3.400 2.900 2.100 peak 5781 weight 0.10000E+01 volume 0.15742E+01 ppm1 7.951 ppm2 0.557
ASSI { 5791}
(( segid "PROT" and resid 87 and name HN ))
(( segid "PROT" and resid 86 and name HG1 ))
3.300 2.700 2.200 peak 5791 weight 0.10000E+01 volume 0.18417E+01 ppm1 7.948 ppm2 1.313
ASSI { 5801}
(( segid "PROT" and resid 107 and name HN ))
(( segid "PROT" and resid 104 and name HA ))
3.100 2.400 2.400 peak 5801 weight 0.10000E+01 volume 0.30498E+01 ppm1 8.404 ppm2 4.086
ASSI { 5811}
(( segid "PROT" and resid 107 and name HN ))
(( segid "PROT" and resid 104 and name HB1 ))
3.500 3.100 2.000 peak 5811 weight 0.10000E+01 volume 0.12855E+01 ppm1 8.404 ppm2 1.940
ASSI { 5821}
(( segid "PROT" and resid 107 and name HN ))
(( segid "PROT" and resid 110 and name HG1 ))
3.600 3.200 1.900 peak 5821 weight 0.10000E+01 volume 0.11312E+01 ppm1 8.402 ppm2 1.128
ASSI { 5831}
(( segid "PROT" and resid 87 and name HN ))
(( segid "PROT" and resid 89 and name HN ))
3.300 2.700 2.200 peak 5831 weight 0.10000E+01 volume 0.20634E+01 ppm1 7.950 ppm2 8.119
ASSI { 5841}
(( segid "PROT" and resid 87 and name HN ))
(( segid "PROT" and resid 85 and name HN ))

```

3.600	3.200	1.900	peak	5841	weight	0.10000E+01	volume	0.11971E+01	ppm1	7.950	ppm2	6.901
ASSI { 5851}												
((segid "PROT" and resid 87 and name HN))												
((segid "PROT" and resid 84 and name HB1))												
3.300	2.700	2.200	peak	5851	weight	0.10000E+01	volume	0.19660E+01	ppm1	7.955	ppm2	3.000
ASSI { 5861}												
((segid "PROT" and resid 87 and name HN))												
((segid "PROT" and resid 87 and name HG1))												
2.800	2.000	2.000	peak	5861	weight	0.10000E+01	volume	0.48232E+01	ppm1	7.950	ppm2	2.414
ASSI { 5871}												
((segid "PROT" and resid 87 and name HN))												
((segid "PROT" and resid 87 and name HB1))												
2.400	1.400	1.400	peak	5871	weight	0.10000E+01	volume	0.11647E+02	ppm1	7.951	ppm2	2.203
ASSI { 5881}												
((segid "PROT" and resid 87 and name HN))												
((segid "PROT" and resid 86 and name HN))												
2.500	1.600	1.600	peak	5881	weight	0.10000E+01	volume	0.98805E+01	ppm1	7.949	ppm2	7.840
ASSI { 5891}												
((segid "PROT" and resid 87 and name HN))												
((segid "PROT" and resid 87 and name HA))												
2.500	1.600	1.600	peak	5891	weight	0.10000E+01	volume	0.97274E+01	ppm1	7.949	ppm2	4.312
ASSI { 5901}												
((segid "PROT" and resid 87 and name HN))												
((segid "PROT" and resid 88 and name HB2))												
3.400	2.900	2.100	peak	5901	weight	0.10000E+01	volume	0.15195E+01	ppm1	7.948	ppm2	2.915
ASSI { 5911}												
((segid "PROT" and resid 115 and name HN))												
((segid "PROT" and resid 114 and name HA1))												
2.400	1.400	1.400	peak	5911	weight	0.10000E+01	volume	0.11986E+02	ppm1	7.733	ppm2	4.230
ASSI { 5921}												
((segid "PROT" and resid 48 and name HN))												
((segid "PROT" and resid 48 and name HA))												
2.700	1.800	1.800	peak	5921	weight	0.10000E+01	volume	0.62082E+01	ppm1	7.731	ppm2	4.097
ASSI { 5931}												
((segid "PROT" and resid 48 and name HN))												
((segid "PROT" and resid 47 and name HN))												
2.700	1.800	1.800	peak	5931	weight	0.10000E+01	volume	0.67305E+01	ppm1	7.724	ppm2	8.464
ASSI { 5951}												
((segid "PROT" and resid 48 and name HN))												
((segid "PROT" and resid 50 and name HN))												
2.800	2.000	2.000	peak	5951	weight	0.10000E+01	volume	0.54418E+01	ppm1	7.729	ppm2	7.953
ASSI { 5961}												
((segid "PROT" and resid 48 and name HN))												
((segid "PROT" and resid 49 and name HN))												
2.300	1.300	1.300	peak	5961	weight	0.10000E+01	volume	0.15564E+02	ppm1	7.724	ppm2	7.117
ASSI { 5971}												
((segid "PROT" and resid 48 and name HN))												
((segid "PROT" and resid 47 and name HB2))												
3.300	2.700	2.200	peak	5971	weight	0.10000E+01	volume	0.18444E+01	ppm1	7.723	ppm2	2.802
ASSI { 5981}												
((segid "PROT" and resid 48 and name HN))												
((segid "PROT" and resid 48 and name HG1))												
2.900	2.100	2.100	peak	5981	weight	0.10000E+01	volume	0.41807E+01	ppm1	7.725	ppm2	2.352
ASSI { 5991}												
((segid "PROT" and resid 48 and name HN))												
((segid "PROT" and resid 48 and name HG2))												
2.700	1.800	1.800	peak	5991	weight	0.10000E+01	volume	0.59443E+01	ppm1	7.724	ppm2	2.247
ASSI { 6001}												
((segid "PROT" and resid 48 and name HN))												
((segid "PROT" and resid 48 and name HB2))												
2.500	1.600	1.600	peak	6001	weight	0.10000E+01	volume	0.10445E+02	ppm1	7.726	ppm2	2.112
ASSI { 6011}												
((segid "PROT" and resid 48 and name HN))												
((segid "PROT" and resid 49 and name HB))												
3.300	2.700	2.200	peak	6011	weight	0.10000E+01	volume	0.19824E+01	ppm1	7.728	ppm2	1.928
ASSI { 6021}												
((segid "PROT" and resid 115 and name HN))												
((segid "PROT" and resid 116 and name HG12))												
3.100	2.400	2.400	peak	6021	weight	0.10000E+01	volume	0.27995E+01	ppm1	7.728	ppm2	0.938
ASSI { 6031}												
((segid "PROT" and resid 48 and name HN))												
((segid "PROT" and resid 47 and name HB1))												
3.600	3.200	1.900	peak	6031	weight	0.10000E+01	volume	0.11030E+01	ppm1	7.722	ppm2	3.212
ASSI { 6041}												
((segid "PROT" and resid 97 and name HN))												
((segid "PROT" and resid 98 and name HN))												
2.800	2.000	2.000	peak	6041	weight	0.10000E+01	volume	0.49406E+01	ppm1	7.962	ppm2	8.467
ASSI { 6051}												
((segid "PROT" and resid 97 and name HN))												
((segid "PROT" and resid 96 and name HN))												
2.800	2.000	2.000	peak	6051	weight	0.10000E+01	volume	0.50772E+01	ppm1	7.963	ppm2	7.365
ASSI { 6061}												
((segid "PROT" and resid 97 and name HN))												
((segid "PROT" and resid 97 and name HA))												
2.600	1.700	1.700	peak	6061	weight	0.10000E+01	volume	0.83858E+01	ppm1	7.961	ppm2	4.212
ASSI { 6071}												
((segid "PROT" and resid 97 and name HN))												
((segid "PROT" and resid 96 and name HA))												
3.400	2.900	2.100	peak	6071	weight	0.10000E+01	volume	0.16577E+01	ppm1	7.963	ppm2	3.810

```

ASSI { 6081}
(( segid "PROT" and resid 97 and name HN ))
(( segid "PROT" and resid 96 and name HB1 ))
3.000 2.200 2.200 peak 6081 weight 0.10000E+01 volume 0.33617E+01 ppm1 7.962 ppm2 3.393
ASSI { 6091}
(( segid "PROT" and resid 97 and name HN ))
(( segid "PROT" and resid 96 and name HB2 ))
3.100 2.400 2.400 peak 6091 weight 0.10000E+01 volume 0.27139E+01 ppm1 7.965 ppm2 2.563
ASSI { 6101}
(( segid "PROT" and resid 97 and name HN ))
(( segid "PROT" and resid 97 and name HB1 ))
2.400 1.400 1.400 peak 6101 weight 0.10000E+01 volume 0.11569E+02 ppm1 7.962 ppm2 2.090
ASSI { 6111}
(( segid "PROT" and resid 97 and name HN ))
(( segid "PROT" and resid 97 and name HG1 ))
2.600 1.700 1.700 peak 6111 weight 0.10000E+01 volume 0.78350E+01 ppm1 7.962 ppm2 1.819
ASSI { 6121}
(( segid "PROT" and resid 97 and name HN ))
(( segid "PROT" and resid 97 and name HG2 ))
3.000 2.200 2.200 peak 6121 weight 0.10000E+01 volume 0.33860E+01 ppm1 7.962 ppm2 1.602
ASSI { 6151}
(( segid "PROT" and resid 59 and name HN ))
(( segid "PROT" and resid 55 and name HN ))
3.300 2.700 2.200 peak 6151 weight 0.10000E+01 volume 0.20861E+01 ppm1 7.884 ppm2 7.380
ASSI { 6161}
(( segid "PROT" and resid 59 and name HN ))
(( segid "PROT" and resid 55 and name HA ))
2.800 2.000 2.000 peak 6161 weight 0.10000E+01 volume 0.54472E+01 ppm1 7.888 ppm2 4.740
ASSI { 6171}
(( segid "PROT" and resid 59 and name HN ))
(( segid "PROT" and resid 59 and name HA ))
2.900 2.100 2.100 peak 6171 weight 0.10000E+01 volume 0.43029E+01 ppm1 7.888 ppm2 4.300
ASSI { 6181}
(( segid "PROT" and resid 59 and name HN ))
(( segid "PROT" and resid 58 and name HA ))
3.300 2.700 2.200 peak 6181 weight 0.10000E+01 volume 0.20113E+01 ppm1 7.887 ppm2 3.855
ASSI { 6191}
(( segid "PROT" and resid 59 and name HN ))
(( segid "PROT" and resid 59 and name HG1 ))
3.000 2.200 2.200 peak 6191 weight 0.10000E+01 volume 0.31885E+01 ppm1 7.887 ppm2 2.640
ASSI { 6201}
(( segid "PROT" and resid 59 and name HN ))
(( segid "PROT" and resid 59 and name HG2 ))
2.900 2.100 2.100 peak 6201 weight 0.10000E+01 volume 0.41094E+01 ppm1 7.887 ppm2 2.523
ASSI { 6211}
(( segid "PROT" and resid 59 and name HN ))
(( segid "PROT" and resid 55 and name HB1 ))
3.300 2.700 2.200 peak 6211 weight 0.10000E+01 volume 0.21032E+01 ppm1 7.887 ppm2 2.409
ASSI { 6221}
(( segid "PROT" and resid 59 and name HN ))
(( segid "PROT" and resid 59 and name HB1 ))
2.800 2.000 2.000 peak 6221 weight 0.10000E+01 volume 0.46693E+01 ppm1 7.887 ppm2 2.117
ASSI { 6231}
(( segid "PROT" and resid 59 and name HN ))
(( segid "PROT" and resid 59 and name HB2 ))
2.900 2.100 2.100 peak 6231 weight 0.10000E+01 volume 0.43295E+01 ppm1 7.887 ppm2 1.894
ASSI { 6241}
(( segid "PROT" and resid 59 and name HN ))
(( segid "PROT" and resid 59 and name HE% ))
3.200 2.600 2.300 peak 6241 weight 0.10000E+01 volume 0.21931E+01 ppm1 7.890 ppm2 1.281
ASSI { 6251}
(( segid "PROT" and resid 59 and name HN ))
(( segid "PROT" and resid 58 and name HG2% ))
2.900 2.100 2.100 peak 6251 weight 0.10000E+01 volume 0.39266E+01 ppm1 7.886 ppm2 1.073
ASSI { 6261}
(( segid "PROT" and resid 59 and name HN ))
(( segid "PROT" and resid 56 and name HD2% ))
3.500 3.100 2.000 peak 6261 weight 0.10000E+01 volume 0.13248E+01 ppm1 7.891 ppm2 0.647
ASSI { 6281}
(( segid "PROT" and resid 59 and name HN ))
(( segid "PROT" and resid 56 and name HA ))
2.900 2.100 2.100 peak 6281 weight 0.10000E+01 volume 0.46129E+01 ppm1 7.887 ppm2 4.067
ASSI { 6311}
(( segid "PROT" and resid 115 and name HN ))
(( segid "PROT" and resid 110 and name HB ))
3.100 2.400 2.400 peak 6311 weight 0.10000E+01 volume 0.26218E+01 ppm1 7.753 ppm2 1.767
ASSI { 6321}
(( segid "PROT" and resid 115 and name HN ))
(( segid "PROT" and resid 115 and name HG ))
2.300 1.300 1.300 peak 6321 weight 0.10000E+01 volume 0.16690E+02 ppm1 7.747 ppm2 1.572
ASSI { 6331}
(( segid "PROT" and resid 115 and name HN ))
(( segid "PROT" and resid 113 and name HB% ))
2.900 2.100 2.100 peak 6331 weight 0.10000E+01 volume 0.44807E+01 ppm1 7.747 ppm2 1.387
ASSI { 6341}
(( segid "PROT" and resid 115 and name HN ))
(( segid "PROT" and resid 116 and name HN ))
2.400 1.400 1.400 peak 6341 weight 0.10000E+01 volume 0.12116E+02 ppm1 7.746 ppm2 7.473
ASSI { 6351}

```

```

(( segid "PROT" and resid 115 and name HN ))
(( segid "PROT" and resid 110 and name HA ))
3.200 2.600 2.300 peak 6351 weight 0.10000E+01 volume 0.23760E+01 ppm1 7.744 ppm2 3.835
ASSI { 6361}
(( segid "PROT" and resid 115 and name HN ))
(( segid "PROT" and resid 110 and name HG2% ))
2.800 2.000 2.000 peak 6361 weight 0.10000E+01 volume 0.49594E+01 ppm1 7.750 ppm2 0.733
ASSI { 6371}
(( segid "PROT" and resid 113 and name HN ))
(( segid "PROT" and resid 114 and name HN ))
2.300 1.300 1.300 peak 6371 weight 0.10000E+01 volume 0.18295E+02 ppm1 7.628 ppm2 7.752
ASSI { 6381}
(( segid "PROT" and resid 113 and name HN ))
(( segid "PROT" and resid 114 and name HA1 ))
3.200 2.600 2.300 peak 6381 weight 0.10000E+01 volume 0.22373E+01 ppm1 7.626 ppm2 4.224
ASSI { 6391}
(( segid "PROT" and resid 113 and name HN ))
(( segid "PROT" and resid 110 and name HA ))
3.600 2.200 2.200 peak 6391 weight 0.10000E+01 volume 0.31767E+01 ppm1 7.627 ppm2 3.841
ASSI { 6401}
(( segid "PROT" and resid 113 and name HN ))
(( segid "PROT" and resid 112 and name HG2 ))
3.300 2.700 2.200 peak 6401 weight 0.10000E+01 volume 0.19652E+01 ppm1 7.629 ppm2 2.228
ASSI { 6411}
(( segid "PROT" and resid 113 and name HN ))
(( segid "PROT" and resid 109 and name HB1 ))
3.400 2.900 2.100 peak 6411 weight 0.10000E+01 volume 0.16895E+01 ppm1 7.627 ppm2 1.755
ASSI { 6421}
(( segid "PROT" and resid 113 and name HN ))
(( segid "PROT" and resid 109 and name HB2 ))
3.100 2.400 2.400 peak 6421 weight 0.10000E+01 volume 0.29609E+01 ppm1 7.630 ppm2 1.554
ASSI { 6441}
(( segid "PROT" and resid 113 and name HN ))
(( segid "PROT" and resid 110 and name HG2% ))
3.600 3.200 1.900 peak 6441 weight 0.10000E+01 volume 0.12178E+01 ppm1 7.626 ppm2 0.742
ASSI { 6451}
(( segid "PROT" and resid 113 and name HN ))
(( segid "PROT" and resid 21 and name HD1% ))
3.400 2.900 2.100 peak 6451 weight 0.10000E+01 volume 0.16502E+01 ppm1 7.627 ppm2 0.640
ASSI { 6471}
(( segid "PROT" and resid 113 and name HN ))
(( segid "PROT" and resid 113 and name HA ))
2.600 1.700 1.700 peak 6471 weight 0.10000E+01 volume 0.87618E+01 ppm1 7.624 ppm2 4.315
ASSI { 6481}
(( segid "PROT" and resid 113 and name HN ))
(( segid "PROT" and resid 112 and name HA ))
2.800 2.000 2.000 peak 6481 weight 0.10000E+01 volume 0.55195E+01 ppm1 7.624 ppm2 3.999
ASSI { 6491}
(( segid "PROT" and resid 113 and name HN ))
(( segid "PROT" and resid 112 and name HG1 ))
3.400 2.900 2.100 peak 6491 weight 0.10000E+01 volume 0.16104E+01 ppm1 7.622 ppm2 2.363
ASSI { 6501}
(( segid "PROT" and resid 113 and name HN ))
(( segid "PROT" and resid 112 and name HB1 ))
2.500 1.600 1.600 peak 6501 weight 0.10000E+01 volume 0.92492E+01 ppm1 7.623 ppm2 2.082
ASSI { 6511}
(( segid "PROT" and resid 113 and name HN ))
(( segid "PROT" and resid 111 and name HB1 ))
3.500 3.100 2.000 peak 6511 weight 0.10000E+01 volume 0.13800E+01 ppm1 7.621 ppm2 1.871
ASSI { 6521}
(( segid "PROT" and resid 113 and name HN ))
(( segid "PROT" and resid 113 and name HB% ))
2.200 1.200 1.200 peak 6521 weight 0.10000E+01 volume 0.21421E+02 ppm1 7.624 ppm2 1.386
ASSI { 6541}
(( segid "PROT" and resid 81 and name HN ))
(( segid "PROT" and resid 77 and name HA ))
3.600 3.200 1.900 peak 6541 weight 0.10000E+01 volume 0.11964E+01 ppm1 7.019 ppm2 4.358
ASSI { 6561}
(( segid "PROT" and resid 104 and name HN ))
(( segid "PROT" and resid 103 and name HN ))
2.700 1.800 1.800 peak 6561 weight 0.10000E+01 volume 0.71341E+01 ppm1 7.178 ppm2 8.061
ASSI { 6581}
(( segid "PROT" and resid 104 and name HN ))
(( segid "PROT" and resid 104 and name HA ))
2.600 1.700 1.700 peak 6581 weight 0.10000E+01 volume 0.74430E+01 ppm1 7.180 ppm2 4.089
ASSI { 6591}
(( segid "PROT" and resid 104 and name HN ))
(( segid "PROT" and resid 101 and name HA ))
3.200 2.600 2.300 peak 6591 weight 0.10000E+01 volume 0.22040E+01 ppm1 7.180 ppm2 3.679
ASSI { 6601}
(( segid "PROT" and resid 104 and name HN ))
(( segid "PROT" and resid 103 and name HA ))
3.200 2.600 2.300 peak 6601 weight 0.10000E+01 volume 0.25243E+01 ppm1 7.178 ppm2 3.191
ASSI { 6611}
(( segid "PROT" and resid 104 and name HN ))
(( segid "PROT" and resid 105 and name HB2 ))
3.300 2.700 2.200 peak 6611 weight 0.10000E+01 volume 0.18405E+01 ppm1 7.178 ppm2 3.075
ASSI { 6621}
(( segid "PROT" and resid 104 and name HN ))

```

```

    (( segid "PROT" and resid 104 and name HB1 ))
    2.300 1.300 1.300 peak 6621 weight 0.10000E+01 volume 0.17956E+02 ppm1 7.180 ppm2 1.952
ASSI { 6631}
    (( segid "PROT" and resid 104 and name HN ))
    (( segid "PROT" and resid 104 and name HD1 ))
    2.600 2.600 1.900 peak 6631 weight 0.10000E+01 volume 0.72669E+01 ppm1 7.181 ppm2 1.714
ASSI { 6641}
    (( segid "PROT" and resid 104 and name HN ))
    (( segid "PROT" and resid 103 and name HB2 ))
    3.200 2.600 2.300 peak 6641 weight 0.10000E+01 volume 0.25289E+01 ppm1 7.178 ppm2 1.307
ASSI { 6661}
    (( segid "PROT" and resid 104 and name HN ))
    (( segid "PROT" and resid 104 and name HG1 ))
    3.100 2.400 2.400 peak 6661 weight 0.10000E+01 volume 0.29965E+01 ppm1 7.176 ppm2 1.534
ASSI { 6671}
    (( segid "PROT" and resid 35 and name HN ))
    (( segid "PROT" and resid 34 and name HA ))
    3.300 2.700 2.200 peak 6671 weight 0.10000E+01 volume 0.19137E+01 ppm1 7.152 ppm2 4.989
ASSI { 6681}
    (( segid "PROT" and resid 35 and name HN ))
    (( segid "PROT" and resid 36 and name HN ))
    2.500 1.600 1.600 peak 6681 weight 0.10000E+01 volume 0.92061E+01 ppm1 7.150 ppm2 7.689
ASSI { 6701}
    (( segid "PROT" and resid 35 and name HN ))
    (( segid "PROT" and resid 35 and name HA ))
    2.800 2.000 2.000 peak 6701 weight 0.10000E+01 volume 0.55220E+01 ppm1 7.152 ppm2 4.315
ASSI { 6711}
    (( segid "PROT" and resid 35 and name HN ))
    (( segid "PROT" and resid 35 and name HG1 ))
    2.500 1.600 1.600 peak 6711 weight 0.10000E+01 volume 0.10122E+02 ppm1 7.152 ppm2 2.867
ASSI { 6721}
    (( segid "PROT" and resid 35 and name HN ))
    (( segid "PROT" and resid 35 and name HB2 ))
    2.500 1.600 1.600 peak 6721 weight 0.10000E+01 volume 0.10214E+02 ppm1 7.152 ppm2 2.210
ASSI { 6741}
    (( segid "PROT" and resid 81 and name HN ))
    (( segid "PROT" and resid 83 and name HN ))
    3.600 3.200 1.900 peak 6741 weight 0.10000E+01 volume 0.11953E+01 ppm1 7.033 ppm2 9.095
ASSI { 6751}
    (( segid "PROT" and resid 81 and name HN ))
    (( segid "PROT" and resid 82 and name HN ))
    2.700 1.800 1.800 peak 6751 weight 0.10000E+01 volume 0.62507E+01 ppm1 7.031 ppm2 6.404
ASSI { 6761}
    (( segid "PROT" and resid 81 and name HN ))
    (( segid "PROT" and resid 81 and name HA ))
    2.900 2.100 2.100 peak 6761 weight 0.10000E+01 volume 0.43231E+01 ppm1 7.032 ppm2 3.104
ASSI { 6771}
    (( segid "PROT" and resid 81 and name HN ))
    (( segid "PROT" and resid 82 and name HB2 ))
    3.500 3.100 2.000 peak 6771 weight 0.10000E+01 volume 0.12809E+01 ppm1 7.033 ppm2 3.003
ASSI { 6791}
    (( segid "PROT" and resid 81 and name HN ))
    (( segid "PROT" and resid 79 and name HB1 ))
    3.300 2.700 2.200 peak 6791 weight 0.10000E+01 volume 0.18620E+01 ppm1 7.035 ppm2 2.189
ASSI { 6801}
    (( segid "PROT" and resid 81 and name HN ))
    (( segid "PROT" and resid 80 and name HB2 ))
    2.900 2.100 2.100 peak 6801 weight 0.10000E+01 volume 0.45127E+01 ppm1 7.035 ppm2 1.944
ASSI { 6811}
    (( segid "PROT" and resid 81 and name HN ))
    (( segid "PROT" and resid 80 and name HG1 ))
    3.200 2.600 2.300 peak 6811 weight 0.10000E+01 volume 0.22692E+01 ppm1 7.034 ppm2 1.764
ASSI { 6831}
    (( segid "PROT" and resid 81 and name HN ))
    (( segid "PROT" and resid 81 and name HG2% ))
    3.000 2.200 2.200 peak 6831 weight 0.10000E+01 volume 0.37030E+01 ppm1 7.031 ppm2 0.139
ASSI { 6851}
    (( segid "PROT" and resid 81 and name HN ))
    (( segid "PROT" and resid 80 and name HA ))
    3.200 2.600 2.300 peak 6851 weight 0.10000E+01 volume 0.23560E+01 ppm1 7.029 ppm2 4.088
ASSI { 6861}
    (( segid "PROT" and resid 81 and name HN ))
    (( segid "PROT" and resid 78 and name HA ))
    3.200 2.600 2.300 peak 6861 weight 0.10000E+01 volume 0.23796E+01 ppm1 7.029 ppm2 3.387
ASSI { 6871}
    (( segid "PROT" and resid 81 and name HN ))
    (( segid "PROT" and resid 81 and name HB ))
    2.600 1.700 1.700 peak 6871 weight 0.10000E+01 volume 0.77216E+01 ppm1 7.029 ppm2 1.435
ASSI { 6881}
    (( segid "PROT" and resid 81 and name HN ))
    (( segid "PROT" and resid 81 and name HG1% ))
    2.500 1.600 1.600 peak 6881 weight 0.10000E+01 volume 0.10928E+02 ppm1 7.029 ppm2 0.480
ASSI { 6891}
    (( segid "PROT" and resid 85 and name HN ))
    (( segid "PROT" and resid 82 and name HN ))
    3.600 3.200 1.900 peak 6891 weight 0.10000E+01 volume 0.12246E+01 ppm1 6.918 ppm2 6.392
ASSI { 6911}
    (( segid "PROT" and resid 85 and name HN ))
    (( segid "PROT" and resid 81 and name HG1% ))

```

3.300	2.700	2.200	peak	6911	weight	0.10000E+01	volume	0.20441E+01	ppm1	6.915	ppm2	0.485
ASSI { 6931}												
((segid "PROT" and resid 31 and name HN))												
((segid "PROT" and resid 102 and name HG))												
3.100	2.400	2.400	peak	6931	weight	0.10000E+01	volume	0.26707E+01	ppm1	7.914	ppm2	1.638
ASSI { 6941}												
((segid "PROT" and resid 31 and name HN))												
((segid "PROT" and resid 28 and name HN))												
3.400	2.900	2.100	peak	6941	weight	0.10000E+01	volume	0.17063E+01	ppm1	7.913	ppm2	7.563
ASSI { 6951}												
((segid "PROT" and resid 31 and name HN))												
((segid "PROT" and resid 32 and name HN))												
2.500	1.600	1.600	peak	6951	weight	0.10000E+01	volume	0.96419E+01	ppm1	7.913	ppm2	7.103
ASSI { 6961}												
((segid "PROT" and resid 31 and name HN))												
((segid "PROT" and resid 30 and name HA))												
3.100	2.400	2.400	peak	6961	weight	0.10000E+01	volume	0.29200E+01	ppm1	7.913	ppm2	4.830
ASSI { 6981}												
((segid "PROT" and resid 31 and name HN))												
((segid "PROT" and resid 28 and name HB1))												
3.200	2.600	2.300	peak	6981	weight	0.10000E+01	volume	0.25210E+01	ppm1	7.913	ppm2	2.999
ASSI { 6991}												
((segid "PROT" and resid 31 and name HN))												
((segid "PROT" and resid 28 and name HB2))												
3.500	3.100	2.000	peak	6991	weight	0.10000E+01	volume	0.12877E+01	ppm1	7.913	ppm2	2.801
ASSI { 7001}												
((segid "PROT" and resid 31 and name HN))												
((segid "PROT" and resid 31 and name HB%))												
2.200	1.200	1.200	peak	7001	weight	0.10000E+01	volume	0.19840E+02	ppm1	7.913	ppm2	1.734
ASSI { 7011}												
((segid "PROT" and resid 31 and name HN))												
((segid "PROT" and resid 102 and name HD1%))												
2.900	2.100	2.100	peak	7011	weight	0.10000E+01	volume	0.43175E+01	ppm1	7.912	ppm2	0.733
ASSI { 7041}												
((segid "PROT" and resid 85 and name HN))												
((segid "PROT" and resid 88 and name HN))												
3.600	3.200	1.900	peak	7041	weight	0.10000E+01	volume	0.11543E+01	ppm1	6.911	ppm2	7.948
ASSI { 7051}												
((segid "PROT" and resid 85 and name HN))												
((segid "PROT" and resid 85 and name HA))												
3.100	2.400	2.400	peak	7051	weight	0.10000E+01	volume	0.29023E+01	ppm1	6.912	ppm2	4.476
ASSI { 7061}												
((segid "PROT" and resid 85 and name HN))												
((segid "PROT" and resid 82 and name HA))												
3.200	2.600	2.300	peak	7061	weight	0.10000E+01	volume	0.23120E+01	ppm1	6.909	ppm2	4.198
ASSI { 7071}												
((segid "PROT" and resid 85 and name HN))												
((segid "PROT" and resid 85 and name HB1))												
2.900	2.100	2.100	peak	7071	weight	0.10000E+01	volume	0.44281E+01	ppm1	6.909	ppm2	3.391
ASSI { 7081}												
((segid "PROT" and resid 85 and name HN))												
((segid "PROT" and resid 85 and name HB2))												
2.700	1.800	1.800	peak	7081	weight	0.10000E+01	volume	0.60371E+01	ppm1	6.909	ppm2	3.075
ASSI { 7101}												
((segid "PROT" and resid 85 and name HN))												
((segid "PROT" and resid 86 and name HN))												
2.800	2.000	2.000	peak	7101	weight	0.10000E+01	volume	0.52021E+01	ppm1	6.907	ppm2	7.827
ASSI { 7111}												
((segid "PROT" and resid 85 and name HN))												
((segid "PROT" and resid 84 and name HA))												
3.300	2.700	2.200	peak	7111	weight	0.10000E+01	volume	0.20680E+01	ppm1	6.905	ppm2	4.314
ASSI { 7121}												
((segid "PROT" and resid 85 and name HN))												
((segid "PROT" and resid 84 and name HB2))												
3.400	2.900	2.100	peak	7121	weight	0.10000E+01	volume	0.15050E+01	ppm1	6.907	ppm2	2.701
ASSI { 7141}												
((segid "PROT" and resid 23 and name HN))												
((segid "PROT" and resid 22 and name HN))												
2.600	1.700	1.700	peak	7141	weight	0.10000E+01	volume	0.76228E+01	ppm1	8.580	ppm2	8.853
ASSI { 7151}												
((segid "PROT" and resid 23 and name HN))												
((segid "PROT" and resid 24 and name HN))												
2.600	1.700	1.700	peak	7151	weight	0.10000E+01	volume	0.82564E+01	ppm1	8.582	ppm2	8.045
ASSI { 7161}												
((segid "PROT" and resid 23 and name HN))												
((segid "PROT" and resid 20 and name HN))												
3.500	3.100	2.000	peak	7161	weight	0.10000E+01	volume	0.13939E+01	ppm1	8.582	ppm2	7.547
ASSI { 7171}												
((segid "PROT" and resid 23 and name HN))												
((segid "PROT" and resid 20 and name HA))												
3.100	2.400	2.400	peak	7171	weight	0.10000E+01	volume	0.28370E+01	ppm1	8.582	ppm2	4.304
ASSI { 7181}												
((segid "PROT" and resid 23 and name HN))												
((segid "PROT" and resid 23 and name HA))												
2.600	1.700	1.700	peak	7181	weight	0.10000E+01	volume	0.82765E+01	ppm1	8.580	ppm2	4.040
ASSI { 7201}												
((segid "PROT" and resid 23 and name HN))												
((segid "PROT" and resid 19 and name HA))												
3.400	2.900	2.100	peak	7201	weight	0.10000E+01	volume	0.15541E+01	ppm1	8.583	ppm2	3.698


```

ASSI { 7211}
(( segid "PROT" and resid 23 and name HN ))
(( segid "PROT" and resid 24 and name HG1 ))
3.500 3.100 2.000 peak 7211 weight 0.10000E+01 volume 0.13521E+01 ppm1 8.578 ppm2 2.858
ASSI { 7221}
(( segid "PROT" and resid 23 and name HN ))
(( segid "PROT" and resid 23 and name HG1 ))
2.800 2.000 2.000 peak 7221 weight 0.10000E+01 volume 0.52073E+01 ppm1 8.578 ppm2 2.576
ASSI { 7231}
(( segid "PROT" and resid 23 and name HN ))
(( segid "PROT" and resid 23 and name HG2 ))
2.700 1.800 1.800 peak 7231 weight 0.10000E+01 volume 0.61263E+01 ppm1 8.580 ppm2 2.460
ASSI { 7241}
(( segid "PROT" and resid 23 and name HN ))
(( segid "PROT" and resid 23 and name HB1 ))
2.400 1.400 1.400 peak 7241 weight 0.10000E+01 volume 0.12017E+02 ppm1 8.581 ppm2 2.344
ASSI { 7251}
(( segid "PROT" and resid 23 and name HN ))
(( segid "PROT" and resid 23 and name HB2 ))
2.500 1.600 1.600 peak 7251 weight 0.10000E+01 volume 0.97676E+01 ppm1 8.580 ppm2 2.235
ASSI { 7261}
(( segid "PROT" and resid 23 and name HN ))
(( segid "PROT" and resid 22 and name HB1 ))
2.800 2.000 2.000 peak 7261 weight 0.10000E+01 volume 0.52458E+01 ppm1 8.580 ppm2 2.102
ASSI { 7271}
(( segid "PROT" and resid 23 and name HN ))
(( segid "PROT" and resid 22 and name HB2 ))
3.000 2.200 2.200 peak 7271 weight 0.10000E+01 volume 0.34592E+01 ppm1 8.579 ppm2 1.709
ASSI { 7281}
(( segid "PROT" and resid 23 and name HN ))
(( segid "PROT" and resid 25 and name HG2% ))
3.300 2.700 2.200 peak 7281 weight 0.10000E+01 volume 0.20526E+01 ppm1 8.581 ppm2 1.028
ASSI { 7291}
(( segid "PROT" and resid 23 and name HN ))
(( segid "PROT" and resid 21 and name HN ))
3.400 2.900 2.100 peak 7291 weight 0.10000E+01 volume 0.17095E+01 ppm1 8.575 ppm2 7.927
ASSI { 7301}
(( segid "PROT" and resid 23 and name HN ))
(( segid "PROT" and resid 21 and name HB ))
3.300 2.700 2.200 peak 7301 weight 0.10000E+01 volume 0.18595E+01 ppm1 8.576 ppm2 1.934
ASSI { 7311}
(( segid "PROT" and resid 110 and name HN ))
(( segid "PROT" and resid 109 and name HN ))
2.600 1.700 1.700 peak 7311 weight 0.10000E+01 volume 0.81388E+01 ppm1 8.123 ppm2 7.965
ASSI { 7321}
(( segid "PROT" and resid 110 and name HN ))
(( segid "PROT" and resid 111 and name HN ))
2.600 1.700 1.700 peak 7321 weight 0.10000E+01 volume 0.90365E+01 ppm1 8.124 ppm2 7.568
ASSI { 7331}
(( segid "PROT" and resid 110 and name HN ))
(( segid "PROT" and resid 109 and name HA ))
3.100 2.400 2.400 peak 7331 weight 0.10000E+01 volume 0.27003E+01 ppm1 8.123 ppm2 4.051
ASSI { 7341}
(( segid "PROT" and resid 110 and name HN ))
(( segid "PROT" and resid 107 and name HA ))
2.600 1.700 1.700 peak 7341 weight 0.10000E+01 volume 0.82467E+01 ppm1 8.123 ppm2 3.835
ASSI { 7351}
(( segid "PROT" and resid 110 and name HN ))
(( segid "PROT" and resid 109 and name HB1 ))
2.600 1.700 1.700 peak 7351 weight 0.10000E+01 volume 0.83498E+01 ppm1 8.124 ppm2 1.760
ASSI { 7361}
(( segid "PROT" and resid 110 and name HN ))
(( segid "PROT" and resid 109 and name HB2 ))
3.100 2.400 2.400 peak 7361 weight 0.10000E+01 volume 0.30691E+01 ppm1 8.123 ppm2 1.556
ASSI { 7371}
(( segid "PROT" and resid 110 and name HN ))
(( segid "PROT" and resid 110 and name HG12% ))
2.600 1.700 1.700 peak 7371 weight 0.10000E+01 volume 0.78805E+01 ppm1 8.124 ppm2 1.117
ASSI { 7381}
(( segid "PROT" and resid 110 and name HN ))
(( segid "PROT" and resid 115 and name HD2% ))
3.200 2.600 2.300 peak 7381 weight 0.10000E+01 volume 0.22974E+01 ppm1 8.124 ppm2 0.800
ASSI { 7391}
(( segid "PROT" and resid 110 and name HN ))
(( segid "PROT" and resid 110 and name HG2% ))
2.600 1.700 1.700 peak 7391 weight 0.10000E+01 volume 0.85494E+01 ppm1 8.123 ppm2 0.665
ASSI { 7401}
(( segid "PROT" and resid 110 and name HN ))
(( segid "PROT" and resid 110 and name HD1% ))
3.000 2.200 2.200 peak 7401 weight 0.10000E+01 volume 0.37184E+01 ppm1 8.124 ppm2 0.546
ASSI { 7411}
(( segid "PROT" and resid 110 and name HN ))
(( segid "PROT" and resid 106 and name HA ))
3.200 2.600 2.300 peak 7411 weight 0.10000E+01 volume 0.24296E+01 ppm1 8.123 ppm2 3.977
ASSI { 7421}
(( segid "PROT" and resid 110 and name HN ))
(( segid "PROT" and resid 109 and name HD1 ))
3.200 2.600 2.300 peak 7421 weight 0.10000E+01 volume 0.21558E+01 ppm1 8.119 ppm2 1.390
ASSI { 7461}

```

```

(( segid "PROT" and resid 86 and name HN ))
(( segid "PROT" and resid 86 and name HA ))
2.900 2.100 2.100 peak 7461 weight 0.10000E+01 volume 0.39371E+01 ppm1 7.829 ppm2 4.228
ASSI { 7471}
(( segid "PROT" and resid 86 and name HN ))
(( segid "PROT" and resid 83 and name HA ))
3.100 2.400 2.400 peak 7471 weight 0.10000E+01 volume 0.26907E+01 ppm1 7.830 ppm2 3.863
ASSI { 7481}
(( segid "PROT" and resid 86 and name HN ))
(( segid "PROT" and resid 85 and name HB2 ))
3.100 2.400 2.400 peak 7481 weight 0.10000E+01 volume 0.28548E+01 ppm1 7.831 ppm2 3.076
ASSI { 7491}
(( segid "PROT" and resid 86 and name HN ))
(( segid "PROT" and resid 86 and name HG1 ))
2.700 1.800 1.800 peak 7491 weight 0.10000E+01 volume 0.63400E+01 ppm1 7.828 ppm2 1.315
ASSI { 7501}
(( segid "PROT" and resid 86 and name HN ))
(( segid "PROT" and resid 86 and name HG2 ))
3.100 2.400 2.400 peak 7501 weight 0.10000E+01 volume 0.29455E+01 ppm1 7.832 ppm2 0.144
ASSI { 7511}
(( segid "PROT" and resid 86 and name HN ))
(( segid "PROT" and resid 85 and name HB1 ))
3.400 2.900 2.100 peak 7511 weight 0.10000E+01 volume 0.16551E+01 ppm1 7.827 ppm2 3.392
ASSI { 7521}
(( segid "PROT" and resid 86 and name HN ))
(( segid "PROT" and resid 86 and name HB1 ))
2.800 2.000 2.000 peak 7521 weight 0.10000E+01 volume 0.57275E+01 ppm1 7.827 ppm2 1.752
ASSI { 7531}
(( segid "PROT" and resid 86 and name HN ))
(( segid "PROT" and resid 99 and name HB% ))
3.100 2.400 2.400 peak 7531 weight 0.10000E+01 volume 0.29669E+01 ppm1 7.826 ppm2 1.647
ASSI { 7541}
(( segid "PROT" and resid 82 and name HN ))
(( segid "PROT" and resid 80 and name HN ))
3.400 2.900 2.100 peak 7541 weight 0.10000E+01 volume 0.15786E+01 ppm1 6.404 ppm2 7.412
ASSI { 7551}
(( segid "PROT" and resid 82 and name HN ))
(( segid "PROT" and resid 82 and name HB2 ))
2.900 2.100 2.100 peak 7551 weight 0.10000E+01 volume 0.41049E+01 ppm1 6.399 ppm2 2.982
ASSI { 7571}
(( segid "PROT" and resid 82 and name HN ))
(( segid "PROT" and resid 99 and name HB% ))
3.600 3.200 1.900 peak 7571 weight 0.10000E+01 volume 0.11485E+01 ppm1 6.394 ppm2 1.629
ASSI { 7581}
(( segid "PROT" and resid 82 and name HN ))
(( segid "PROT" and resid 79 and name HA ))
3.100 2.400 2.400 peak 7581 weight 0.10000E+01 volume 0.26091E+01 ppm1 6.405 ppm2 3.834
ASSI { 7591}
(( segid "PROT" and resid 82 and name HN ))
(( segid "PROT" and resid 83 and name HN ))
2.700 1.800 1.800 peak 7591 weight 0.10000E+01 volume 0.67167E+01 ppm1 6.398 ppm2 9.087
ASSI { 7611}
(( segid "PROT" and resid 82 and name HN ))
(( segid "PROT" and resid 82 and name HA ))
3.000 2.200 2.200 peak 7611 weight 0.10000E+01 volume 0.35557E+01 ppm1 6.402 ppm2 4.182
ASSI { 7621}
(( segid "PROT" and resid 82 and name HN ))
(( segid "PROT" and resid 81 and name HA ))
2.900 2.100 2.100 peak 7621 weight 0.10000E+01 volume 0.42652E+01 ppm1 6.401 ppm2 3.098
ASSI { 7661}
(( segid "PROT" and resid 82 and name HN ))
(( segid "PROT" and resid 81 and name HB ))
2.700 1.800 1.800 peak 7661 weight 0.10000E+01 volume 0.65677E+01 ppm1 6.398 ppm2 1.437
ASSI { 7681}
(( segid "PROT" and resid 82 and name HN ))
(( segid "PROT" and resid 81 and name HG1% ))
3.100 2.400 2.400 peak 7681 weight 0.10000E+01 volume 0.28381E+01 ppm1 6.396 ppm2 0.485
ASSI { 7691}
(( segid "PROT" and resid 82 and name HN ))
(( segid "PROT" and resid 81 and name HG2% ))
3.000 2.200 2.200 peak 7691 weight 0.10000E+01 volume 0.35300E+01 ppm1 6.401 ppm2 0.132
ASSI { 7701}
(( segid "PROT" and resid 67 and name HN ))
(( segid "PROT" and resid 62 and name HA ))
3.600 3.200 1.900 peak 7701 weight 0.10000E+01 volume 0.10882E+01 ppm1 8.249 ppm2 3.932
ASSI { 7711}
(( segid "PROT" and resid 67 and name HN ))
(( segid "PROT" and resid 68 and name HN ))
2.600 1.700 1.700 peak 7711 weight 0.10000E+01 volume 0.79629E+01 ppm1 8.244 ppm2 8.011
ASSI { 7721}
(( segid "PROT" and resid 67 and name HN ))
(( segid "PROT" and resid 63 and name HA ))
3.100 2.400 2.400 peak 7721 weight 0.10000E+01 volume 0.28926E+01 ppm1 8.243 ppm2 4.736
ASSI { 7731}
(( segid "PROT" and resid 67 and name HN ))
(( segid "PROT" and resid 66 and name HA ))
2.900 2.100 2.100 peak 7731 weight 0.10000E+01 volume 0.40872E+01 ppm1 8.243 ppm2 4.413
ASSI { 7741}
(( segid "PROT" and resid 67 and name HN ))

```

```

    (( segid "PROT" and resid 67 and name HA ))
    2.800 2.000 2.000 peak 7741 weight 0.10000E+01 volume 0.48819E+01 ppm1 8.243 ppm2 4.080
ASSI { 7751}
    (( segid "PROT" and resid 67 and name HN ))
    (( segid "PROT" and resid 67 and name HB1 ))
    2.600 1.700 1.700 peak 7751 weight 0.10000E+01 volume 0.73162E+01 ppm1 8.244 ppm2 2.976
ASSI { 7761}
    (( segid "PROT" and resid 67 and name HN ))
    (( segid "PROT" and resid 65 and name HB2 ))
    3.300 2.700 2.200 peak 7761 weight 0.10000E+01 volume 0.19397E+01 ppm1 8.244 ppm2 2.777
ASSI { 7771}
    (( segid "PROT" and resid 67 and name HN ))
    (( segid "PROT" and resid 67 and name HB2 ))
    2.600 1.700 1.700 peak 7771 weight 0.10000E+01 volume 0.79008E+01 ppm1 8.244 ppm2 2.065
ASSI { 7781}
    (( segid "PROT" and resid 67 and name HN ))
    (( segid "PROT" and resid 62 and name HB2 ))
    3.400 2.900 2.100 peak 7781 weight 0.10000E+01 volume 0.17159E+01 ppm1 8.245 ppm2 1.104
ASSI { 7791}
    (( segid "PROT" and resid 67 and name HN ))
    (( segid "PROT" and resid 69 and name HG1% ))
    3.600 3.200 1.900 peak 7791 weight 0.10000E+01 volume 0.11159E+01 ppm1 8.245 ppm2 0.985
ASSI { 7831}
    (( segid "PROT" and resid 98 and name HN ))
    (( segid "PROT" and resid 99 and name HN ))
    2.700 1.800 1.800 peak 7831 weight 0.10000E+01 volume 0.67297E+01 ppm1 8.468 ppm2 8.193
ASSI { 7861}
    (( segid "PROT" and resid 98 and name HN ))
    (( segid "PROT" and resid 98 and name HA ))
    2.700 1.800 1.800 peak 7861 weight 0.10000E+01 volume 0.70923E+01 ppm1 8.469 ppm2 4.203
ASSI { 7871}
    (( segid "PROT" and resid 98 and name HN ))
    (( segid "PROT" and resid 98 and name HB1 ))
    2.900 2.100 2.100 peak 7871 weight 0.10000E+01 volume 0.40399E+01 ppm1 8.463 ppm2 3.387
ASSI { 7881}
    (( segid "PROT" and resid 98 and name HN ))
    (( segid "PROT" and resid 98 and name HB2 ))
    2.700 1.800 1.800 peak 7881 weight 0.10000E+01 volume 0.60660E+01 ppm1 8.465 ppm2 3.031
ASSI { 7891}
    (( segid "PROT" and resid 98 and name HN ))
    (( segid "PROT" and resid 97 and name HG2 ))
    3.200 2.600 2.300 peak 7891 weight 0.10000E+01 volume 0.22366E+01 ppm1 8.469 ppm2 1.629
ASSI { 7911}
    (( segid "PROT" and resid 98 and name HN ))
    (( segid "PROT" and resid 96 and name HN ))
    3.200 2.600 2.300 peak 7911 weight 0.10000E+01 volume 0.25397E+01 ppm1 8.436 ppm2 7.377
ASSI { 7921}
    (( segid "PROT" and resid 52 and name HN ))
    (( segid "PROT" and resid 50 and name HA ))
    3.000 2.200 2.200 peak 7921 weight 0.10000E+01 volume 0.36881E+01 ppm1 8.430 ppm2 3.923
ASSI { 7931}
    (( segid "PROT" and resid 52 and name HN ))
    (( segid "PROT" and resid 53 and name HD1 ))
    3.200 2.600 2.300 peak 7931 weight 0.10000E+01 volume 0.21891E+01 ppm1 8.437 ppm2 3.634
ASSI { 7941}
    (( segid "PROT" and resid 52 and name HN ))
    (( segid "PROT" and resid 52 and name HB2 ))
    2.700 1.800 1.800 peak 7941 weight 0.10000E+01 volume 0.71866E+01 ppm1 8.431 ppm2 2.936
ASSI { 7961}
    (( segid "PROT" and resid 52 and name HN ))
    (( segid "PROT" and resid 52 and name HD% ))
    3.300 2.700 2.200 peak 7961 weight 0.10000E+01 volume 0.20400E+01 ppm1 8.426 ppm2 7.245
ASSI { 7971}
    (( segid "PROT" and resid 52 and name HN ))
    (( segid "PROT" and resid 52 and name HA ))
    2.800 2.000 2.000 peak 7971 weight 0.10000E+01 volume 0.47172E+01 ppm1 8.427 ppm2 5.013
ASSI { 7981}
    (( segid "PROT" and resid 52 and name HN ))
    (( segid "PROT" and resid 51 and name HA ))
    2.900 2.100 2.100 peak 7981 weight 0.10000E+01 volume 0.44512E+01 ppm1 8.430 ppm2 3.854
ASSI { 7991}
    (( segid "PROT" and resid 52 and name HN ))
    (( segid "PROT" and resid 51 and name HG1 ))
    2.900 2.100 2.100 peak 7991 weight 0.10000E+01 volume 0.40272E+01 ppm1 8.428 ppm2 1.365
ASSI { 8001}
    (( segid "PROT" and resid 52 and name HN ))
    (( segid "PROT" and resid 51 and name HG2 ))
    2.800 2.000 2.000 peak 8001 weight 0.10000E+01 volume 0.48060E+01 ppm1 8.429 ppm2 1.183
ASSI { 8011}
    (( segid "PROT" and resid 52 and name HN ))
    (( segid "PROT" and resid 50 and name HG2% ))
    2.700 1.800 1.800 peak 8011 weight 0.10000E+01 volume 0.57798E+01 ppm1 8.430 ppm2 0.391
ASSI { 8031}
    (( segid "PROT" and resid 32 and name HN ))
    (( segid "PROT" and resid 29 and name HA ))
    3.500 3.100 2.000 peak 8031 weight 0.10000E+01 volume 0.14468E+01 ppm1 7.101 ppm2 4.239
ASSI { 8041}
    (( segid "PROT" and resid 32 and name HN ))
    (( segid "PROT" and resid 102 and name HD1% ))

```

```

3.500    3.100    2.000 peak 8041 weight 0.10000E+01 volume 0.14091E+01 ppm1 7.098 ppm2 0.734
ASSI { 8051}
(( segid "PROT" and resid 75 and name HN ))
(( segid "PROT" and resid 74 and name HD% ))
3.400    2.900    2.100 peak 8051 weight 0.10000E+01 volume 0.15423E+01 ppm1 8.509 ppm2 6.405
ASSI { 8061}
(( segid "PROT" and resid 75 and name HN ))
(( segid "PROT" and resid 72 and name HA ))
3.000    2.200    2.200 peak 8061 weight 0.10000E+01 volume 0.36517E+01 ppm1 8.502 ppm2 4.063
ASSI { 8071}
(( segid "PROT" and resid 75 and name HN ))
(( segid "PROT" and resid 74 and name HA ))
3.200    2.600    2.300 peak 8071 weight 0.10000E+01 volume 0.23481E+01 ppm1 8.494 ppm2 3.791
ASSI { 8081}
(( segid "PROT" and resid 75 and name HN ))
(( segid "PROT" and resid 73 and name HB2 ))
3.400    2.900    2.100 peak 8081 weight 0.10000E+01 volume 0.16840E+01 ppm1 8.486 ppm2 1.891
ASSI { 8091}
(( segid "PROT" and resid 98 and name HN ))
(( segid "PROT" and resid 97 and name HB1 ))
2.600    1.700    1.700 peak 8091 weight 0.10000E+01 volume 0.73028E+01 ppm1 8.473 ppm2 2.090
ASSI { 8101}
(( segid "PROT" and resid 98 and name HN ))
(( segid "PROT" and resid 97 and name HG1 ))
3.200    2.600    2.300 peak 8101 weight 0.10000E+01 volume 0.22962E+01 ppm1 8.471 ppm2 1.827
ASSI { 8111}
(( segid "PROT" and resid 95 and name HN ))
(( segid "PROT" and resid 96 and name HN ))
3.600    3.200    1.900 peak 8111 weight 0.10000E+01 volume 0.11106E+01 ppm1 7.966 ppm2 7.391
ASSI { 8121}
(( segid "PROT" and resid 60 and name HN ))
(( segid "PROT" and resid 60 and name HA ))
2.700    1.800    1.800 peak 8121 weight 0.10000E+01 volume 0.60698E+01 ppm1 7.963 ppm2 4.414
ASSI { 8131}
(( segid "PROT" and resid 95 and name HN ))
(( segid "PROT" and resid 94 and name HA ))
2.600    1.700    1.700 peak 8131 weight 0.10000E+01 volume 0.76180E+01 ppm1 7.963 ppm2 4.222
ASSI { 8141}
(( segid "PROT" and resid 60 and name HN ))
(( segid "PROT" and resid 61 and name HG1 ))
3.200    2.600    2.300 peak 8141 weight 0.10000E+01 volume 0.23031E+01 ppm1 7.959 ppm2 2.382
ASSI { 8151}
(( segid "PROT" and resid 65 and name HN ))
(( segid "PROT" and resid 63 and name HB2 ))
3.000    2.200    2.200 peak 8151 weight 0.10000E+01 volume 0.34813E+01 ppm1 7.961 ppm2 1.915
ASSI { 8161}
(( segid "PROT" and resid 65 and name HN ))
(( segid "PROT" and resid 62 and name HB2 ))
2.900    2.100    2.100 peak 8161 weight 0.10000E+01 volume 0.42507E+01 ppm1 7.963 ppm2 1.076
ASSI { 8171}
(( segid "PROT" and resid 65 and name HN ))
(( segid "PROT" and resid 62 and name HG2 ))
3.600    3.200    1.900 peak 8171 weight 0.10000E+01 volume 0.11342E+01 ppm1 7.965 ppm2 0.891
ASSI { 8191}
(( segid "PROT" and resid 88 and name HN ))
(( segid "PROT" and resid 88 and name HA ))
2.600    1.700    1.700 peak 8191 weight 0.10000E+01 volume 0.74064E+01 ppm1 7.940 ppm2 4.309
ASSI { 8201}
(( segid "PROT" and resid 88 and name HN ))
(( segid "PROT" and resid 88 and name HB1 ))
2.800    2.000    2.000 peak 8201 weight 0.10000E+01 volume 0.50457E+01 ppm1 7.943 ppm2 2.936
ASSI { 8211}
(( segid "PROT" and resid 88 and name HN ))
(( segid "PROT" and resid 87 and name HB1 ))
2.900    2.100    2.100 peak 8211 weight 0.10000E+01 volume 0.46367E+01 ppm1 7.948 ppm2 2.198
ASSI { 8221}
(( segid "PROT" and resid 88 and name HN ))
(( segid "PROT" and resid 50 and name HD1% ))
3.200    2.600    2.300 peak 8221 weight 0.10000E+01 volume 0.21507E+01 ppm1 7.940 ppm2 0.559
ASSI { 8241}
(( segid "PROT" and resid 32 and name HN ))
(( segid "PROT" and resid 32 and name HE1 ))
3.400    2.900    2.100 peak 8241 weight 0.10000E+01 volume 0.15718E+01 ppm1 7.101 ppm2 10.403
ASSI { 8271}
(( segid "PROT" and resid 32 and name HN ))
(( segid "PROT" and resid 30 and name HA ))
3.500    3.100    2.000 peak 8271 weight 0.10000E+01 volume 0.12594E+01 ppm1 7.102 ppm2 4.829
ASSI { 8281}
(( segid "PROT" and resid 32 and name HN ))
(( segid "PROT" and resid 32 and name HA ))
2.700    1.800    1.800 peak 8281 weight 0.10000E+01 volume 0.68837E+01 ppm1 7.101 ppm2 4.399
ASSI { 8291}
(( segid "PROT" and resid 32 and name HN ))
(( segid "PROT" and resid 32 and name HB1 ))
2.900    2.100    2.100 peak 8291 weight 0.10000E+01 volume 0.43852E+01 ppm1 7.100 ppm2 3.614
ASSI { 8301}
(( segid "PROT" and resid 32 and name HN ))
(( segid "PROT" and resid 32 and name HB2 ))
2.700    1.800    1.800 peak 8301 weight 0.10000E+01 volume 0.59584E+01 ppm1 7.099 ppm2 3.384

```

```

ASSI { 8311}
  (( segid "PROT" and resid 32 and name HN ))
  (( segid "PROT" and resid 35 and name HB2 ))
  3.300 2.700 2.200 peak 8311 weight 0.10000E+01 volume 0.21134E+01 ppm1 7.100 ppm2 2.216
ASSI { 8321}
  (( segid "PROT" and resid 32 and name HN ))
  (( segid "PROT" and resid 31 and name HB2 ))
  2.800 2.000 2.000 peak 8321 weight 0.10000E+01 volume 0.49211E+01 ppm1 7.100 ppm2 1.734
ASSI { 8331}
  (( segid "PROT" and resid 32 and name HN ))
  (( segid "PROT" and resid 33 and name HD2 ))
  3.000 2.200 2.200 peak 8331 weight 0.10000E+01 volume 0.36037E+01 ppm1 7.101 ppm2 1.553
ASSI { 8341}
  (( segid "PROT" and resid 32 and name HN ))
  (( segid "PROT" and resid 34 and name HN ))
  3.500 3.100 2.000 peak 8341 weight 0.10000E+01 volume 0.13342E+01 ppm1 7.093 ppm2 7.630
ASSI { 8351}
  (( segid "PROT" and resid 56 and name HN ))
  (( segid "PROT" and resid 56 and name HB2 ))
  3.200 2.600 2.300 peak 8351 weight 0.10000E+01 volume 0.22617E+01 ppm1 9.137 ppm2 1.417
ASSI { 8361}
  (( segid "PROT" and resid 56 and name HN ))
  (( segid "PROT" and resid 56 and name HD18 ))
  3.200 2.600 2.300 peak 8361 weight 0.10000E+01 volume 0.21571E+01 ppm1 9.136 ppm2 0.952
ASSI { 8371}
  (( segid "PROT" and resid 75 and name HN ))
  (( segid "PROT" and resid 76 and name HN ))
  2.600 1.700 1.700 peak 8371 weight 0.10000E+01 volume 0.76502E+01 ppm1 8.504 ppm2 8.021
ASSI { 8421}
  (( segid "PROT" and resid 75 and name HN ))
  (( segid "PROT" and resid 75 and name HB1 ))
  2.600 1.700 1.700 peak 8421 weight 0.10000E+01 volume 0.88439E+01 ppm1 8.504 ppm2 2.947
ASSI { 8431}
  (( segid "PROT" and resid 75 and name HN ))
  (( segid "PROT" and resid 75 and name HB2 ))
  2.900 2.100 2.100 peak 8431 weight 0.10000E+01 volume 0.41666E+01 ppm1 8.504 ppm2 2.619
ASSI { 8441}
  (( segid "PROT" and resid 75 and name HN ))
  (( segid "PROT" and resid 75 and name HG1 ))
  2.800 2.000 2.000 peak 8441 weight 0.10000E+01 volume 0.47167E+01 ppm1 8.506 ppm2 2.322
ASSI { 8451}
  (( segid "PROT" and resid 75 and name HN ))
  (( segid "PROT" and resid 75 and name HG2 ))
  2.700 1.800 1.800 peak 8451 weight 0.10000E+01 volume 0.59655E+01 ppm1 8.507 ppm2 2.221
ASSI { 8471}
  (( segid "PROT" and resid 60 and name HN ))
  (( segid "PROT" and resid 63 and name HN ))
  3.300 2.700 2.200 peak 8471 weight 0.10000E+01 volume 0.18372E+01 ppm1 7.966 ppm2 8.884
ASSI { 8481}
  (( segid "PROT" and resid 65 and name HN ))
  (( segid "PROT" and resid 62 and name HN ))
  3.600 3.200 1.900 peak 8481 weight 0.10000E+01 volume 0.12461E+01 ppm1 7.958 ppm2 8.376
ASSI { 8491}
  (( segid "PROT" and resid 60 and name HN ))
  (( segid "PROT" and resid 61 and name HN ))
  2.300 1.300 1.300 peak 8491 weight 0.10000E+01 volume 0.16597E+02 ppm1 7.963 ppm2 8.166
ASSI { 8501}
  (( segid "PROT" and resid 65 and name HN ))
  (( segid "PROT" and resid 65 and name HD21 ))
  3.100 2.400 2.400 peak 8501 weight 0.10000E+01 volume 0.29272E+01 ppm1 7.960 ppm2 7.603
ASSI { 8511}
  (( segid "PROT" and resid 65 and name HN ))
  (( segid "PROT" and resid 65 and name HD22 ))
  3.300 2.700 2.200 peak 8511 weight 0.10000E+01 volume 0.20934E+01 ppm1 7.960 ppm2 6.977
ASSI { 8521}
  (( segid "PROT" and resid 65 and name HN ))
  (( segid "PROT" and resid 65 and name HA ))
  2.700 1.800 1.800 peak 8521 weight 0.10000E+01 volume 0.69853E+01 ppm1 7.962 ppm2 4.805
ASSI { 8531}
  (( segid "PROT" and resid 95 and name HN ))
  (( segid "PROT" and resid 93 and name HA ))
  3.400 2.900 2.100 peak 8531 weight 0.10000E+01 volume 0.17105E+01 ppm1 7.962 ppm2 4.527
ASSI { 8541}
  (( segid "PROT" and resid 60 and name HN ))
  (( segid "PROT" and resid 60 and name HB2 ))
  2.700 1.800 1.800 peak 8541 weight 0.10000E+01 volume 0.68005E+01 ppm1 7.963 ppm2 4.059
ASSI { 8551}
  (( segid "PROT" and resid 65 and name HN ))
  (( segid "PROT" and resid 62 and name HA ))
  3.100 2.400 2.400 peak 8551 weight 0.10000E+01 volume 0.28044E+01 ppm1 7.963 ppm2 3.886
ASSI { 8571}
  (( segid "PROT" and resid 65 and name HN ))
  (( segid "PROT" and resid 65 and name HB2 ))
  2.500 1.600 1.600 peak 8571 weight 0.10000E+01 volume 0.98965E+01 ppm1 7.961 ppm2 2.786
ASSI { 8581}
  (( segid "PROT" and resid 65 and name HN ))
  (( segid "PROT" and resid 64 and name HB1 ))
  2.500 1.600 1.600 peak 8581 weight 0.10000E+01 volume 0.10932E+02 ppm1 7.960 ppm2 2.061
ASSI { 8611}

```

```

(( segid "PROT" and resid 65 and name HN ))
(( segid "PROT" and resid 65 and name HB1 ))
2.600 1.700 1.700 peak 8611 weight 0.10000E+01 volume 0.86756E+01 ppm1 7.958 ppm2 3.027
ASSI { 8621}
(( segid "PROT" and resid 56 and name HN ))
(( segid "PROT" and resid 34 and name HB1 ))
3.500 3.100 2.000 peak 8621 weight 0.10000E+01 volume 0.13755E+01 ppm1 9.138 ppm2 3.495
ASSI { 8631}
(( segid "PROT" and resid 56 and name HN ))
(( segid "PROT" and resid 56 and name HB1 ))
3.100 2.400 2.400 peak 8631 weight 0.10000E+01 volume 0.27193E+01 ppm1 9.139 ppm2 2.074
ASSI { 8651}
(( segid "PROT" and resid 56 and name HN ))
(( segid "PROT" and resid 55 and name HA ))
2.800 2.000 2.000 peak 8651 weight 0.10000E+01 volume 0.49101E+01 ppm1 9.133 ppm2 4.746
ASSI { 8661}
(( segid "PROT" and resid 56 and name HN ))
(( segid "PROT" and resid 35 and name HA ))
3.500 3.100 2.000 peak 8661 weight 0.10000E+01 volume 0.12922E+01 ppm1 9.134 ppm2 4.311
ASSI { 8671}
(( segid "PROT" and resid 56 and name HN ))
(( segid "PROT" and resid 56 and name HA ))
3.300 2.700 2.200 peak 8671 weight 0.10000E+01 volume 0.20678E+01 ppm1 9.134 ppm2 4.038
ASSI { 8681}
(( segid "PROT" and resid 56 and name HN ))
(( segid "PROT" and resid 55 and name HB1 ))
2.800 2.000 2.000 peak 8681 weight 0.10000E+01 volume 0.49656E+01 ppm1 9.136 ppm2 2.380
ASSI { 8691}
(( segid "PROT" and resid 56 and name HN ))
(( segid "PROT" and resid 56 and name HG ))
2.800 2.000 2.000 peak 8691 weight 0.10000E+01 volume 0.48001E+01 ppm1 9.133 ppm2 1.733
ASSI { 8711}
(( segid "PROT" and resid 56 and name HN ))
(( segid "PROT" and resid 56 and name HD2% ))
3.100 2.400 2.400 peak 8711 weight 0.10000E+01 volume 0.28913E+01 ppm1 9.137 ppm2 0.647
ASSI { 8721}
(( segid "PROT" and resid 56 and name HN ))
(( segid "PROT" and resid 81 and name HG1% ))
3.600 3.200 1.900 peak 8721 weight 0.10000E+01 volume 0.11502E+01 ppm1 9.131 ppm2 0.486
ASSI { 8751}
(( segid "PROT" and resid 69 and name HN ))
(( segid "PROT" and resid 68 and name HA ))
2.600 1.700 1.700 peak 8751 weight 0.10000E+01 volume 0.87535E+01 ppm1 7.703 ppm2 4.550
ASSI { 8761}
(( segid "PROT" and resid 69 and name HN ))
(( segid "PROT" and resid 69 and name HA ))
2.800 2.000 2.000 peak 8761 weight 0.10000E+01 volume 0.55954E+01 ppm1 7.703 ppm2 4.099
ASSI { 8771}
(( segid "PROT" and resid 69 and name HN ))
(( segid "PROT" and resid 69 and name HB ))
3.100 2.400 2.400 peak 8771 weight 0.10000E+01 volume 0.25963E+01 ppm1 7.705 ppm2 2.334
ASSI { 8781}
(( segid "PROT" and resid 69 and name HN ))
(( segid "PROT" and resid 69 and name HG1% ))
2.300 1.300 1.300 peak 8781 weight 0.10000E+01 volume 0.15076E+02 ppm1 7.703 ppm2 0.960
ASSI { 8791}
(( segid "PROT" and resid 69 and name HN ))
(( segid "PROT" and resid 69 and name HG2% ))
2.400 1.400 1.400 peak 8791 weight 0.10000E+01 volume 0.14135E+02 ppm1 7.703 ppm2 0.840
ASSI { 8801}
(( segid "PROT" and resid 69 and name HN ))
(( segid "PROT" and resid 68 and name HB2 ))
3.500 3.100 2.000 peak 8801 weight 0.10000E+01 volume 0.13700E+01 ppm1 7.697 ppm2 2.922
ASSI { 8811}
(( segid "PROT" and resid 93 and name HN ))
(( segid "PROT" and resid 90 and name HD1 ))
3.400 2.900 2.100 peak 8811 weight 0.10000E+01 volume 0.14810E+01 ppm1 8.123 ppm2 4.101
ASSI { 8821}
(( segid "PROT" and resid 93 and name HN ))
(( segid "PROT" and resid 92 and name HG2 ))
3.100 2.400 2.400 peak 8821 weight 0.10000E+01 volume 0.27236E+01 ppm1 8.117 ppm2 2.231
ASSI { 8831}
(( segid "PROT" and resid 93 and name HN ))
(( segid "PROT" and resid 94 and name HN ))
2.600 1.700 1.700 peak 8831 weight 0.10000E+01 volume 0.72426E+01 ppm1 8.122 ppm2 8.399
ASSI { 8841}
(( segid "PROT" and resid 93 and name HN ))
(( segid "PROT" and resid 90 and name HA ))
3.400 2.900 2.100 peak 8841 weight 0.10000E+01 volume 0.15414E+01 ppm1 8.126 ppm2 4.634
ASSI { 8851}
(( segid "PROT" and resid 93 and name HN ))
(( segid "PROT" and resid 93 and name HA ))
2.800 2.000 2.000 peak 8851 weight 0.10000E+01 volume 0.47169E+01 ppm1 8.123 ppm2 4.498
ASSI { 8861}
(( segid "PROT" and resid 93 and name HN ))
(( segid "PROT" and resid 96 and name HA ))
3.600 3.200 1.900 peak 8861 weight 0.10000E+01 volume 0.12225E+01 ppm1 8.131 ppm2 3.813
ASSI { 8871}
(( segid "PROT" and resid 93 and name HN ))

```

```

(( segid "PROT" and resid 96 and name HB1 ))
3.200 2.600 2.300 peak 8871 weight 0.10000E+01 volume 0.22127E+01 ppm1 8.121 ppm2 3.389
ASSI { 8881}
(( segid "PROT" and resid 93 and name HN ))
(( segid "PROT" and resid 96 and name HB2 ))
3.200 2.600 2.300 peak 8881 weight 0.10000E+01 volume 0.22961E+01 ppm1 8.122 ppm2 2.561
ASSI { 8891}
(( segid "PROT" and resid 93 and name HN ))
(( segid "PROT" and resid 96 and name HN ))
3.500 3.100 2.000 peak 8891 weight 0.10000E+01 volume 0.13954E+01 ppm1 8.120 ppm2 7.358
ASSI { 8901}
(( segid "PROT" and resid 93 and name HN ))
(( segid "PROT" and resid 92 and name HA ))
2.700 1.800 1.800 peak 8901 weight 0.10000E+01 volume 0.59769E+01 ppm1 8.118 ppm2 4.240
ASSI { 8911}
(( segid "PROT" and resid 93 and name HN ))
(( segid "PROT" and resid 92 and name HB1 ))
2.900 2.100 2.100 peak 8911 weight 0.10000E+01 volume 0.38660E+01 ppm1 8.118 ppm2 2.079
ASSI { 8921}
(( segid "PROT" and resid 100 and name HN ))
(( segid "PROT" and resid 98 and name HN ))
3.400 2.900 2.100 peak 8921 weight 0.10000E+01 volume 0.15387E+01 ppm1 8.078 ppm2 8.500
ASSI { 8941}
(( segid "PROT" and resid 100 and name HN ))
(( segid "PROT" and resid 97 and name HA ))
2.800 2.000 2.000 peak 8941 weight 0.10000E+01 volume 0.50553E+01 ppm1 8.076 ppm2 4.216
ASSI { 8951}
(( segid "PROT" and resid 100 and name HN ))
(( segid "PROT" and resid 99 and name HA ))
3.200 2.600 2.300 peak 8951 weight 0.10000E+01 volume 0.21329E+01 ppm1 8.075 ppm2 3.886
ASSI { 8961}
(( segid "PROT" and resid 100 and name HN ))
(( segid "PROT" and resid 96 and name HA ))
3.500 3.100 2.000 peak 8961 weight 0.10000E+01 volume 0.13805E+01 ppm1 8.072 ppm2 3.815
ASSI { 8971}
(( segid "PROT" and resid 100 and name HN ))
(( segid "PROT" and resid 100 and name HB2 ))
2.500 1.600 1.600 peak 8971 weight 0.10000E+01 volume 0.11200E+02 ppm1 8.073 ppm2 2.819
ASSI { 8981}
(( segid "PROT" and resid 100 and name HN ))
(( segid "PROT" and resid 101 and name HB ))
3.400 2.900 2.100 peak 8981 weight 0.10000E+01 volume 0.16226E+01 ppm1 8.072 ppm2 1.924
ASSI { 8991}
(( segid "PROT" and resid 100 and name HN ))
(( segid "PROT" and resid 103 and name HB1 ))
3.400 2.900 2.100 peak 8991 weight 0.10000E+01 volume 0.16128E+01 ppm1 8.074 ppm2 1.798
ASSI { 9001}
(( segid "PROT" and resid 100 and name HN ))
(( segid "PROT" and resid 100 and name HA ))
2.600 1.700 1.700 peak 9001 weight 0.10000E+01 volume 0.77227E+01 ppm1 8.070 ppm2 4.336
ASSI { 9011}
(( segid "PROT" and resid 100 and name HN ))
(( segid "PROT" and resid 100 and name HB1 ))
2.600 1.700 1.700 peak 9011 weight 0.10000E+01 volume 0.85998E+01 ppm1 8.070 ppm2 2.902
ASSI { 9021}
(( segid "PROT" and resid 100 and name HN ))
(( segid "PROT" and resid 99 and name HB* ))
2.600 1.700 1.700 peak 9021 weight 0.10000E+01 volume 0.72646E+01 ppm1 8.070 ppm2 1.633
ASSI { 9031}
(( segid "PROT" and resid 83 and name HN ))
(( segid "PROT" and resid 81 and name HA ))
3.100 2.400 2.400 peak 9031 weight 0.10000E+01 volume 0.27010E+01 ppm1 9.097 ppm2 3.099
ASSI { 9051}
(( segid "PROT" and resid 83 and name HN ))
(( segid "PROT" and resid 79 and name HE21 ))
3.500 3.100 2.000 peak 9051 weight 0.10000E+01 volume 0.12887E+01 ppm1 9.097 ppm2 7.316
ASSI { 9081}
(( segid "PROT" and resid 83 and name HN ))
(( segid "PROT" and resid 83 and name HB ))
2.800 2.000 2.000 peak 9081 weight 0.10000E+01 volume 0.50910E+01 ppm1 9.095 ppm2 4.211
ASSI { 9091}
(( segid "PROT" and resid 83 and name HN ))
(( segid "PROT" and resid 80 and name HA ))
3.000 2.200 2.200 peak 9091 weight 0.10000E+01 volume 0.37309E+01 ppm1 9.094 ppm2 4.081
ASSI { 9101}
(( segid "PROT" and resid 83 and name HN ))
(( segid "PROT" and resid 83 and name HA ))
2.800 2.000 2.000 peak 9101 weight 0.10000E+01 volume 0.47850E+01 ppm1 9.095 ppm2 3.866
ASSI { 9111}
(( segid "PROT" and resid 83 and name HN ))
(( segid "PROT" and resid 82 and name HB2 ))
3.000 2.200 2.200 peak 9111 weight 0.10000E+01 volume 0.35514E+01 ppm1 9.096 ppm2 2.980
ASSI { 9121}
(( segid "PROT" and resid 83 and name HN ))
(( segid "PROT" and resid 83 and name HG2* ))
2.600 1.700 1.700 peak 9121 weight 0.10000E+01 volume 0.77238E+01 ppm1 9.096 ppm2 1.319
ASSI { 9171}
(( segid "PROT" and resid 116 and name HN ))
(( segid "PROT" and resid 115 and name HA ))

```

```

2.500 1.600 1.600 peak 9171 weight 0.10000E+01 volume 0.10961E+02 ppm1 7.472 ppm2 4.243
ASSI { 9181}
(( segid "PROT" and resid 116 and name HN ))
(( segid "PROT" and resid 111 and name HA ))
2.900 2.100 2.100 peak 9181 weight 0.10000E+01 volume 0.41946E+01 ppm1 7.472 ppm2 4.067
ASSI { 9191}
(( segid "PROT" and resid 116 and name HN ))
(( segid "PROT" and resid 116 and name HB ))
2.600 1.700 1.700 peak 9191 weight 0.10000E+01 volume 0.82844E+01 ppm1 7.473 ppm2 1.827
ASSI { 9201}
(( segid "PROT" and resid 116 and name HN ))
(( segid "PROT" and resid 115 and name HG ))
2.800 2.000 2.000 peak 9201 weight 0.10000E+01 volume 0.52666E+01 ppm1 7.472 ppm2 1.582
ASSI { 9211}
(( segid "PROT" and resid 116 and name HN ))
(( segid "PROT" and resid 116 and name HG11))
2.800 2.000 2.000 peak 9211 weight 0.10000E+01 volume 0.51800E+01 ppm1 7.472 ppm2 1.326
ASSI { 9221}
(( segid "PROT" and resid 116 and name HN ))
(( segid "PROT" and resid 116 and name HG12))
2.700 1.800 1.800 peak 9221 weight 0.10000E+01 volume 0.61501E+01 ppm1 7.472 ppm2 0.937
ASSI { 9231}
(( segid "PROT" and resid 116 and name HN ))
(( segid "PROT" and resid 116 and name HD1*))
2.800 2.000 2.000 peak 9231 weight 0.10000E+01 volume 0.56999E+01 ppm1 7.472 ppm2 0.822
ASSI { 9241}
(( segid "PROT" and resid 116 and name HN ))
(( segid "PROT" and resid 110 and name HG2*))
3.400 2.900 2.100 peak 9241 weight 0.10000E+01 volume 0.16152E+01 ppm1 7.474 ppm2 0.683
ASSI { 9261}
(( segid "PROT" and resid 89 and name HN ))
(( segid "PROT" and resid 89 and name HD21))
3.000 2.200 2.200 peak 9261 weight 0.10000E+01 volume 0.33062E+01 ppm1 8.116 ppm2 8.355
ASSI { 9271}
(( segid "PROT" and resid 89 and name HN ))
(( segid "PROT" and resid 88 and name HN ))
2.600 1.700 1.700 peak 9271 weight 0.10000E+01 volume 0.81545E+01 ppm1 8.115 ppm2 7.938
ASSI { 9281}
(( segid "PROT" and resid 89 and name HN ))
(( segid "PROT" and resid 86 and name HN ))
3.100 2.400 2.400 peak 9281 weight 0.10000E+01 volume 0.30920E+01 ppm1 8.119 ppm2 7.822
ASSI { 9291}
(( segid "PROT" and resid 89 and name HN ))
(( segid "PROT" and resid 86 and name HA ))
3.400 2.900 2.100 peak 9291 weight 0.10000E+01 volume 0.15463E+01 ppm1 8.113 ppm2 4.229
ASSI { 9301}
(( segid "PROT" and resid 89 and name HN ))
(( segid "PROT" and resid 89 and name HB1 ))
2.900 2.100 2.100 peak 9301 weight 0.10000E+01 volume 0.37959E+01 ppm1 8.117 ppm2 3.068
ASSI { 9311}
(( segid "PROT" and resid 89 and name HN ))
(( segid "PROT" and resid 89 and name HA ))
3.100 2.400 2.400 peak 9311 weight 0.10000E+01 volume 0.27926E+01 ppm1 8.111 ppm2 5.063
ASSI { 9321}
(( segid "PROT" and resid 89 and name HN ))
(( segid "PROT" and resid 87 and name HA ))
3.300 2.700 2.200 peak 9321 weight 0.10000E+01 volume 0.20761E+01 ppm1 8.111 ppm2 4.307
ASSI { 9331}
(( segid "PROT" and resid 89 and name HN ))
(( segid "PROT" and resid 89 and name HB2 ))
2.800 2.000 2.000 peak 9331 weight 0.10000E+01 volume 0.50152E+01 ppm1 8.112 ppm2 2.891
ASSI { 9341}
(( segid "PROT" and resid 108 and name HN ))
(( segid "PROT" and resid 110 and name HN ))
2.900 2.100 2.100 peak 9341 weight 0.10000E+01 volume 0.40916E+01 ppm1 7.945 ppm2 8.119
ASSI { 9351}
(( segid "PROT" and resid 108 and name HN ))
(( segid "PROT" and resid 107 and name HN ))
2.500 1.600 1.600 peak 9351 weight 0.10000E+01 volume 0.95030E+01 ppm1 7.934 ppm2 8.399
ASSI { 9361}
(( segid "PROT" and resid 108 and name HN ))
(( segid "PROT" and resid 105 and name HA ))
3.100 2.400 2.400 peak 9361 weight 0.10000E+01 volume 0.29117E+01 ppm1 7.935 ppm2 4.336
ASSI { 9371}
(( segid "PROT" and resid 108 and name HN ))
(( segid "PROT" and resid 104 and name HA ))
2.900 2.100 2.100 peak 9371 weight 0.10000E+01 volume 0.44614E+01 ppm1 7.935 ppm2 4.086
ASSI { 9381}
(( segid "PROT" and resid 108 and name HN ))
(( segid "PROT" and resid 107 and name HB1 ))
2.600 1.700 1.700 peak 9381 weight 0.10000E+01 volume 0.86992E+01 ppm1 7.934 ppm2 3.071
ASSI { 9391}
(( segid "PROT" and resid 108 and name HN ))
(( segid "PROT" and resid 108 and name HA ))
2.700 1.800 1.800 peak 9391 weight 0.10000E+01 volume 0.69670E+01 ppm1 7.933 ppm2 4.207
ASSI { 9401}
(( segid "PROT" and resid 108 and name HN ))
(( segid "PROT" and resid 108 and name HB1 ))
2.300 1.300 1.300 peak 9401 weight 0.10000E+01 volume 0.15144E+02 ppm1 7.933 ppm2 3.994

```



```

ASSI { 9411}
  (( segid "PROT" and resid 108 and name HN ))
  (( segid "PROT" and resid 107 and name HA ))
  3.000 2.200 2.200 peak 9411 weight 0.10000E+01 volume 0.36835E+01 ppm1 7.931 ppm2 3.856
ASSI { 9431}
  (( segid "PROT" and resid 108 and name HN ))
  (( segid "PROT" and resid 109 and name HG1 ))
  3.500 3.100 2.000 peak 9431 weight 0.10000E+01 volume 0.14551E+01 ppm1 7.928 ppm2 0.819
ASSI { 9441}
  (( segid "PROT" and resid 49 and name HN ))
  (( segid "PROT" and resid 50 and name HB ))
  3.500 3.100 2.000 peak 9441 weight 0.10000E+01 volume 0.14054E+01 ppm1 7.116 ppm2 1.212
ASSI { 9471}
  (( segid "PROT" and resid 49 and name HN ))
  (( segid "PROT" and resid 48 and name HA ))
  2.800 2.000 2.000 peak 9471 weight 0.10000E+01 volume 0.50132E+01 ppm1 7.114 ppm2 4.092
ASSI { 9481}
  (( segid "PROT" and resid 49 and name HN ))
  (( segid "PROT" and resid 48 and name HB2 ))
  3.000 2.200 2.200 peak 9481 weight 0.10000E+01 volume 0.32610E+01 ppm1 7.114 ppm2 2.104
ASSI { 9491}
  (( segid "PROT" and resid 49 and name HN ))
  (( segid "PROT" and resid 49 and name HB ))
  2.900 2.100 2.100 peak 9491 weight 0.10000E+01 volume 0.39099E+01 ppm1 7.113 ppm2 1.909
ASSI { 9501}
  (( segid "PROT" and resid 49 and name HN ))
  (( segid "PROT" and resid 49 and name HG1% ))
  2.600 1.700 1.700 peak 9501 weight 0.10000E+01 volume 0.78825E+01 ppm1 7.115 ppm2 0.938
ASSI { 9531}
  (( segid "PROT" and resid 68 and name HN ))
  (( segid "PROT" and resid 69 and name HN ))
  3.300 2.700 2.200 peak 9531 weight 0.10000E+01 volume 0.19914E+01 ppm1 8.008 ppm2 7.709
ASSI { 9561}
  (( segid "PROT" and resid 68 and name HN ))
  (( segid "PROT" and resid 63 and name HA ))
  2.800 2.000 2.000 peak 9561 weight 0.10000E+01 volume 0.51283E+01 ppm1 8.010 ppm2 4.736
ASSI { 9571}
  (( segid "PROT" and resid 68 and name HN ))
  (( segid "PROT" and resid 68 and name HA ))
  3.000 2.200 2.200 peak 9571 weight 0.10000E+01 volume 0.33992E+01 ppm1 8.012 ppm2 4.545
ASSI { 9581}
  (( segid "PROT" and resid 68 and name HN ))
  (( segid "PROT" and resid 66 and name HA ))
  3.200 2.600 2.300 peak 9581 weight 0.10000E+01 volume 0.25061E+01 ppm1 8.007 ppm2 4.406
ASSI { 9591}
  (( segid "PROT" and resid 68 and name HN ))
  (( segid "PROT" and resid 67 and name HA ))
  3.200 2.600 2.300 peak 9591 weight 0.10000E+01 volume 0.22241E+01 ppm1 8.008 ppm2 4.080
ASSI { 9601}
  (( segid "PROT" and resid 68 and name HN ))
  (( segid "PROT" and resid 68 and name HB1 ))
  2.700 1.800 1.800 peak 9601 weight 0.10000E+01 volume 0.64844E+01 ppm1 8.010 ppm2 3.066
ASSI { 9611}
  (( segid "PROT" and resid 68 and name HN ))
  (( segid "PROT" and resid 68 and name HB2 ))
  2.800 2.000 2.000 peak 9611 weight 0.10000E+01 volume 0.52689E+01 ppm1 8.013 ppm2 2.942
ASSI { 9621}
  (( segid "PROT" and resid 68 and name HN ))
  (( segid "PROT" and resid 62 and name HB1 ))
  3.000 2.200 2.200 peak 9621 weight 0.10000E+01 volume 0.34737E+01 ppm1 8.012 ppm2 2.069
ASSI { 9631}
  (( segid "PROT" and resid 68 and name HN ))
  (( segid "PROT" and resid 62 and name HB2 ))
  3.300 2.700 2.200 peak 9631 weight 0.10000E+01 volume 0.20544E+01 ppm1 8.009 ppm2 1.048
ASSI { 9641}
  (( segid "PROT" and resid 68 and name HN ))
  (( segid "PROT" and resid 62 and name HG2 ))
  3.500 3.100 2.000 peak 9641 weight 0.10000E+01 volume 0.13121E+01 ppm1 8.009 ppm2 0.839
ASSI { 9661}
  (( segid "PROT" and resid 68 and name HN ))
  (( segid "PROT" and resid 73 and name HD1% ))
  3.300 2.700 2.200 peak 9661 weight 0.10000E+01 volume 0.18934E+01 ppm1 8.006 ppm2 0.968
ASSI { 9671}
  (( segid "PROT" and resid 49 and name HN ))
  (( segid "PROT" and resid 46 and name HA ))
  3.600 3.200 1.900 peak 9671 weight 0.10000E+01 volume 0.11481E+01 ppm1 7.104 ppm2 3.480
ASSI { 9681}
  (( segid "PROT" and resid 26 and name HN ))
  (( segid "PROT" and resid 24 and name HN ))
  3.600 3.200 1.900 peak 9681 weight 0.10000E+01 volume 0.11188E+01 ppm1 8.577 ppm2 8.046
ASSI { 9691}
  (( segid "PROT" and resid 26 and name HN ))
  (( segid "PROT" and resid 28 and name HN ))
  2.700 1.800 1.800 peak 9691 weight 0.10000E+01 volume 0.58413E+01 ppm1 8.577 ppm2 7.555
ASSI { 9701}
  (( segid "PROT" and resid 26 and name HN ))
  (( segid "PROT" and resid 25 and name HB ))
  2.800 2.000 2.000 peak 9701 weight 0.10000E+01 volume 0.48076E+01 ppm1 8.580 ppm2 2.409
ASSI { 9711}

```

```

(( segid "PROT" and resid 26 and name HN ))
(( segid "PROT" and resid 26 and name HB1 ))
2.500 1.600 1.600 peak 9711 weight 0.10000E+01 volume 0.10862E+02 ppm1 8.577 ppm2 1.885
ASSI { 9721}
(( segid "PROT" and resid 26 and name HN ))
(( segid "PROT" and resid 26 and name HG1 ))
3.200 2.600 2.300 peak 9721 weight 0.10000E+01 volume 0.25005E+01 ppm1 8.578 ppm2 1.503
ASSI { 9731}
(( segid "PROT" and resid 26 and name HN ))
(( segid "PROT" and resid 25 and name HG2% ))
2.900 2.100 2.100 peak 9731 weight 0.10000E+01 volume 0.41014E+01 ppm1 8.577 ppm2 1.032
ASSI { 9741}
(( segid "PROT" and resid 26 and name HN ))
(( segid "PROT" and resid 23 and name HA ))
3.000 2.200 2.200 peak 9741 weight 0.10000E+01 volume 0.36360E+01 ppm1 8.575 ppm2 4.040
ASSI { 9751}
(( segid "PROT" and resid 26 and name HN ))
(( segid "PROT" and resid 26 and name HA ))
2.800 2.000 2.000 peak 9751 weight 0.10000E+01 volume 0.51742E+01 ppm1 8.575 ppm2 3.899
ASSI { 9761}
(( segid "PROT" and resid 26 and name HN ))
(( segid "PROT" and resid 28 and name HB2 ))
3.300 2.700 2.200 peak 9761 weight 0.10000E+01 volume 0.17856E+01 ppm1 8.571 ppm2 2.822
ASSI { 9771}
(( segid "PROT" and resid 26 and name HN ))
(( segid "PROT" and resid 22 and name HB2 ))
3.200 2.600 2.300 peak 9771 weight 0.10000E+01 volume 0.24703E+01 ppm1 8.574 ppm2 1.720
ASSI { 9781}
(( segid "PROT" and resid 26 and name HN ))
(( segid "PROT" and resid 25 and name HG1% ))
3.200 2.600 2.300 peak 9781 weight 0.10000E+01 volume 0.21814E+01 ppm1 8.575 ppm2 1.204
ASSI { 9791}
(( segid "PROT" and resid 68 and name HN ))
(( segid "PROT" and resid 68 and name HD% ))
3.400 2.900 2.100 peak 9791 weight 0.10000E+01 volume 0.17151E+01 ppm1 8.012 ppm2 7.177
ASSI { 9811}
(( segid "PROT" and resid 66 and name HN ))
(( segid "PROT" and resid 66 and name HB2 ))
2.900 2.100 2.100 peak 9811 weight 0.10000E+01 volume 0.45427E+01 ppm1 8.165 ppm2 2.064
ASSI { 9821}
(( segid "PROT" and resid 66 and name HN ))
(( segid "PROT" and resid 65 and name HN ))
2.500 1.600 1.600 peak 9821 weight 0.10000E+01 volume 0.94679E+01 ppm1 8.167 ppm2 7.964
ASSI { 9831}
(( segid "PROT" and resid 66 and name HN ))
(( segid "PROT" and resid 65 and name HA ))
3.100 2.400 2.400 peak 9831 weight 0.10000E+01 volume 0.29187E+01 ppm1 8.168 ppm2 4.805
ASSI { 9841}
(( segid "PROT" and resid 66 and name HN ))
(( segid "PROT" and resid 63 and name HA ))
2.900 2.100 2.100 peak 9841 weight 0.10000E+01 volume 0.39314E+01 ppm1 8.166 ppm2 4.740
ASSI { 9851}
(( segid "PROT" and resid 66 and name HN ))
(( segid "PROT" and resid 66 and name HA ))
2.400 1.400 1.400 peak 9851 weight 0.10000E+01 volume 0.12932E+02 ppm1 8.168 ppm2 4.413
ASSI { 9881}
(( segid "PROT" and resid 66 and name HN ))
(( segid "PROT" and resid 66 and name HG2 ))
2.900 2.100 2.100 peak 9881 weight 0.10000E+01 volume 0.40718E+01 ppm1 8.168 ppm2 1.558
ASSI { 9891}
(( segid "PROT" and resid 66 and name HN ))
(( segid "PROT" and resid 65 and name HB2 ))
3.400 2.900 2.100 peak 9891 weight 0.10000E+01 volume 0.16398E+01 ppm1 8.160 ppm2 2.783
ASSI { 9901}
(( segid "PROT" and resid 79 and name HN ))
(( segid "PROT" and resid 80 and name HN ))
2.300 1.300 1.300 peak 9901 weight 0.10000E+01 volume 0.14943E+02 ppm1 8.099 ppm2 7.402
ASSI { 9911}
(( segid "PROT" and resid 79 and name HN ))
(( segid "PROT" and resid 81 and name HN ))
3.300 2.700 2.200 peak 9911 weight 0.10000E+01 volume 0.18162E+01 ppm1 8.097 ppm2 7.043
ASSI { 9921}
(( segid "PROT" and resid 79 and name HN ))
(( segid "PROT" and resid 75 and name HA ))
3.100 2.400 2.400 peak 9921 weight 0.10000E+01 volume 0.26898E+01 ppm1 8.100 ppm2 4.089
ASSI { 9941}
(( segid "PROT" and resid 79 and name HN ))
(( segid "PROT" and resid 79 and name HA ))
2.700 1.800 1.800 peak 9941 weight 0.10000E+01 volume 0.59060E+01 ppm1 8.098 ppm2 3.824
ASSI { 9951}
(( segid "PROT" and resid 79 and name HN ))
(( segid "PROT" and resid 78 and name HA ))
3.400 2.900 2.100 peak 9951 weight 0.10000E+01 volume 0.17317E+01 ppm1 8.102 ppm2 3.388
ASSI { 9961}
(( segid "PROT" and resid 79 and name HN ))
(( segid "PROT" and resid 79 and name HG1 ))
2.800 2.000 2.000 peak 9961 weight 0.10000E+01 volume 0.52811E+01 ppm1 8.100 ppm2 2.455
ASSI { 9971}
(( segid "PROT" and resid 79 and name HN ))

```

```

(( segid "PROT" and resid 79 and name HB1 ))
2.500 1.600 1.600 peak 9971 weight 0.10000E+01 volume 0.10887E+02 ppm1 8.099 ppm2 2.184
ASSI { 9981}
(( segid "PROT" and resid 79 and name HN ))
(( segid "PROT" and resid 79 and name HB2 ))
2.500 1.600 1.600 peak 9981 weight 0.10000E+01 volume 0.95335E+01 ppm1 8.101 ppm2 2.088
ASSI { 9991}
(( segid "PROT" and resid 79 and name HN ))
(( segid "PROT" and resid 78 and name HB1 ))
2.900 2.100 2.100 peak 9991 weight 0.10000E+01 volume 0.38537E+01 ppm1 8.096 ppm2 0.720
ASSI {10001}
(( segid "PROT" and resid 79 and name HN ))
(( segid "PROT" and resid 78 and name HB2 ))
3.100 2.400 2.400 peak 10001 weight 0.10000E+01 volume 0.25858E+01 ppm1 8.098 ppm2 0.451
ASSI {10011}
(( segid "PROT" and resid 79 and name HN ))
(( segid "PROT" and resid 78 and name HD1 ))
3.500 3.100 2.000 peak 10011 weight 0.10000E+01 volume 0.13409E+01 ppm1 8.094 ppm2 0.067
ASSI {10021}
(( segid "PROT" and resid 36 and name HN ))
(( segid "PROT" and resid 56 and name HN ))
3.500 3.100 2.000 peak 10021 weight 0.10000E+01 volume 0.12688E+01 ppm1 7.690 ppm2 9.127
ASSI {10041}
(( segid "PROT" and resid 36 and name HN ))
(( segid "PROT" and resid 34 and name HA ))
3.500 3.100 2.000 peak 10041 weight 0.10000E+01 volume 0.13356E+01 ppm1 7.691 ppm2 4.975
ASSI {10051}
(( segid "PROT" and resid 36 and name HN ))
(( segid "PROT" and resid 36 and name HA ))
2.700 1.800 1.800 peak 10051 weight 0.10000E+01 volume 0.61193E+01 ppm1 7.691 ppm2 4.846
ASSI {10061}
(( segid "PROT" and resid 36 and name HN ))
(( segid "PROT" and resid 55 and name HA ))
3.000 2.200 2.200 peak 10061 weight 0.10000E+01 volume 0.33550E+01 ppm1 7.693 ppm2 4.744
ASSI {10071}
(( segid "PROT" and resid 36 and name HN ))
(( segid "PROT" and resid 35 and name HA ))
3.000 2.200 2.200 peak 10071 weight 0.10000E+01 volume 0.33318E+01 ppm1 7.692 ppm2 4.310
ASSI {10081}
(( segid "PROT" and resid 36 and name HN ))
(( segid "PROT" and resid 36 and name HG1 ))
2.400 1.400 1.400 peak 10081 weight 0.10000E+01 volume 0.12415E+02 ppm1 7.692 ppm2 2.186
ASSI {10091}
(( segid "PROT" and resid 36 and name HN ))
(( segid "PROT" and resid 36 and name HB2 ))
2.600 1.700 1.700 peak 10091 weight 0.10000E+01 volume 0.75637E+01 ppm1 7.691 ppm2 1.775
ASSI {10101}
(( segid "PROT" and resid 36 and name HN ))
(( segid "PROT" and resid 57 and name HN ))
3.600 3.200 1.900 peak 10101 weight 0.10000E+01 volume 0.11945E+01 ppm1 7.686 ppm2 8.787
ASSI {10111}
(( segid "PROT" and resid 36 and name HN ))
(( segid "PROT" and resid 37 and name HD1 ))
3.300 2.700 2.200 peak 10111 weight 0.10000E+01 volume 0.19817E+01 ppm1 7.685 ppm2 3.675
ASSI {10121}
(( segid "PROT" and resid 36 and name HN ))
(( segid "PROT" and resid 35 and name HG1 ))
3.400 2.900 2.100 peak 10121 weight 0.10000E+01 volume 0.16945E+01 ppm1 7.688 ppm2 2.874
ASSI {10131}
(( segid "PROT" and resid 47 and name HN ))
(( segid "PROT" and resid 53 and name HD1 ))
3.200 2.600 2.300 peak 10131 weight 0.10000E+01 volume 0.23466E+01 ppm1 8.421 ppm2 3.609
ASSI {10151}
(( segid "PROT" and resid 94 and name HN ))
(( segid "PROT" and resid 94 and name HA ))
2.600 1.700 1.700 peak 10151 weight 0.10000E+01 volume 0.75591E+01 ppm1 8.402 ppm2 4.230
ASSI {10161}
(( segid "PROT" and resid 94 and name HN ))
(( segid "PROT" and resid 96 and name HB2 ))
3.000 2.200 2.200 peak 10161 weight 0.10000E+01 volume 0.31379E+01 ppm1 8.397 ppm2 2.566
ASSI {10171}
(( segid "PROT" and resid 94 and name HN ))
(( segid "PROT" and resid 90 and name HB1 ))
3.200 2.600 2.300 peak 10171 weight 0.10000E+01 volume 0.22427E+01 ppm1 8.405 ppm2 2.336
ASSI {10181}
(( segid "PROT" and resid 94 and name HN ))
(( segid "PROT" and resid 94 and name HG1 ))
2.600 1.700 1.700 peak 10181 weight 0.10000E+01 volume 0.83426E+01 ppm1 8.401 ppm2 2.236
ASSI {10201}
(( segid "PROT" and resid 94 and name HN ))
(( segid "PROT" and resid 94 and name HB2 ))
2.500 1.600 1.600 peak 10201 weight 0.10000E+01 volume 0.92976E+01 ppm1 8.402 ppm2 1.989
ASSI {10211}
(( segid "PROT" and resid 94 and name HN ))
(( segid "PROT" and resid 97 and name HG1 ))
3.600 3.200 1.900 peak 10211 weight 0.10000E+01 volume 0.12042E+01 ppm1 8.403 ppm2 1.853
ASSI {10231}
(( segid "PROT" and resid 20 and name HN ))
(( segid "PROT" and resid 22 and name HN ))

```

3.300	2.700	2.200	peak 10231	weight	0.10000E+01	volume	0.19933E+01	ppm1	7.546	ppm2	8.853
ASSI {10241}											
((segid "PROT" and resid 20 and name HN))											
((segid "PROT" and resid 19 and name HN))											
2.500	1.600	1.600	peak 10241	weight	0.10000E+01	volume	0.93544E+01	ppm1	7.545	ppm2	8.569
ASSI {10251}											
((segid "PROT" and resid 20 and name HN))											
((segid "PROT" and resid 21 and name HN))											
2.500	1.600	1.600	peak 10251	weight	0.10000E+01	volume	0.94546E+01	ppm1	7.546	ppm2	7.924
ASSI {10261}											
((segid "PROT" and resid 20 and name HN))											
((segid "PROT" and resid 18 and name HN))											
3.300	2.700	2.200	peak 10261	weight	0.10000E+01	volume	0.18399E+01	ppm1	7.547	ppm2	8.489
ASSI {10281}											
((segid "PROT" and resid 20 and name HN))											
((segid "PROT" and resid 20 and name HA))											
2.600	1.700	1.700	peak 10281	weight	0.10000E+01	volume	0.89922E+01	ppm1	7.547	ppm2	4.302
ASSI {10291}											
((segid "PROT" and resid 20 and name HN))											
((segid "PROT" and resid 16 and name HA))											
2.900	2.100	2.100	peak 10291	weight	0.10000E+01	volume	0.38903E+01	ppm1	7.547	ppm2	4.188
ASSI {10301}											
((segid "PROT" and resid 20 and name HN))											
((segid "PROT" and resid 20 and name HB1))											
2.200	1.200	1.200	peak 10301	weight	0.10000E+01	volume	0.20909E+02	ppm1	7.546	ppm2	4.077
ASSI {10311}											
((segid "PROT" and resid 20 and name HN))											
((segid "PROT" and resid 17 and name HA))											
2.700	1.800	1.800	peak 10311	weight	0.10000E+01	volume	0.67614E+01	ppm1	7.547	ppm2	3.948
ASSI {10321}											
((segid "PROT" and resid 20 and name HN))											
((segid "PROT" and resid 21 and name HA))											
3.400	2.900	2.100	peak 10321	weight	0.10000E+01	volume	0.17488E+01	ppm1	7.547	ppm2	3.788
ASSI {10331}											
((segid "PROT" and resid 20 and name HN))											
((segid "PROT" and resid 21 and name HB))											
3.400	2.900	2.100	peak 10331	weight	0.10000E+01	volume	0.16067E+01	ppm1	7.546	ppm2	1.925
ASSI {10341}											
((segid "PROT" and resid 20 and name HN))											
((segid "PROT" and resid 19 and name HB1))											
2.600	1.700	1.700	peak 10341	weight	0.10000E+01	volume	0.76773E+01	ppm1	7.545	ppm2	1.708
ASSI {10351}											
((segid "PROT" and resid 20 and name HN))											
((segid "PROT" and resid 19 and name HB2))											
2.900	2.100	2.100	peak 10351	weight	0.10000E+01	volume	0.42261E+01	ppm1	7.546	ppm2	1.379
ASSI {10361}											
((segid "PROT" and resid 20 and name HN))											
((segid "PROT" and resid 19 and name HG1))											
2.900	2.100	2.100	peak 10361	weight	0.10000E+01	volume	0.44504E+01	ppm1	7.547	ppm2	1.283
ASSI {10371}											
((segid "PROT" and resid 20 and name HN))											
((segid "PROT" and resid 17 and name HG2))											
3.400	2.900	2.100	peak 10371	weight	0.10000E+01	volume	0.15554E+01	ppm1	7.549	ppm2	1.166
ASSI {10391}											
((segid "PROT" and resid 20 and name HN))											
((segid "PROT" and resid 19 and name HA))											
3.000	2.200	2.200	peak 10391	weight	0.10000E+01	volume	0.34252E+01	ppm1	7.543	ppm2	3.696
ASSI {10401}											
((segid "PROT" and resid 20 and name HN))											
((segid "PROT" and resid 21 and name HG12))											
3.300	2.700	2.200	peak 10401	weight	0.10000E+01	volume	0.17938E+01	ppm1	7.542	ppm2	1.039
ASSI {10411}											
((segid "PROT" and resid 34 and name HN))											
((segid "PROT" and resid 35 and name HN))											
2.300	1.300	1.300	peak 10411	weight	0.10000E+01	volume	0.15055E+02	ppm1	7.612	ppm2	7.150
ASSI {10421}											
((segid "PROT" and resid 34 and name HN))											
((segid "PROT" and resid 34 and name HA))											
3.000	2.200	2.200	peak 10421	weight	0.10000E+01	volume	0.34973E+01	ppm1	7.614	ppm2	4.977
ASSI {10431}											
((segid "PROT" and resid 34 and name HN))											
((segid "PROT" and resid 32 and name HA))											
3.200	2.600	2.300	peak 10431	weight	0.10000E+01	volume	0.22167E+01	ppm1	7.615	ppm2	4.402
ASSI {10441}											
((segid "PROT" and resid 34 and name HN))											
((segid "PROT" and resid 34 and name HB1))											
3.000	2.200	2.200	peak 10441	weight	0.10000E+01	volume	0.31345E+01	ppm1	7.614	ppm2	3.488
ASSI {10451}											
((segid "PROT" and resid 34 and name HN))											
((segid "PROT" and resid 35 and name HG1))											
3.100	2.400	2.400	peak 10451	weight	0.10000E+01	volume	0.30809E+01	ppm1	7.612	ppm2	2.867
ASSI {10461}											
((segid "PROT" and resid 34 and name HN))											
((segid "PROT" and resid 34 and name HB2))											
2.800	2.000	2.000	peak 10461	weight	0.10000E+01	volume	0.48777E+01	ppm1	7.612	ppm2	2.596
ASSI {10471}											
((segid "PROT" and resid 34 and name HN))											
((segid "PROT" and resid 33 and name HD1))											
2.900	2.100	2.100	peak 10471	weight	0.10000E+01	volume	0.40744E+01	ppm1	7.614	ppm2	2.227

```

ASSI {10481}
  (( segid "PROT" and resid 34 and name HN ))
  (( segid "PROT" and resid 56 and name HG ))
  3.200 2.600 2.300 peak 10481 weight 0.10000E+01 volume 0.22953E+01 ppm1 7.611 ppm2 1.734
ASSI {10491}
  (( segid "PROT" and resid 34 and name HN ))
  (( segid "PROT" and resid 33 and name HD2 ))
  3.400 2.900 2.100 peak 10491 weight 0.10000E+01 volume 0.17403E+01 ppm1 7.613 ppm2 1.555
ASSI {10501}
  (( segid "PROT" and resid 34 and name HN ))
  (( segid "PROT" and resid 33 and name HB1 ))
  3.400 2.900 2.100 peak 10501 weight 0.10000E+01 volume 0.15736E+01 ppm1 7.611 ppm2 1.022
ASSI {10521}
  (( segid "PROT" and resid 34 and name HN ))
  (( segid "PROT" and resid 81 and name HG2% ))
  3.500 3.100 2.000 peak 10521 weight 0.10000E+01 volume 0.13578E+01 ppm1 7.614 ppm2 0.128
ASSI {10531}
  (( segid "PROT" and resid 34 and name HN ))
  (( segid "PROT" and resid 33 and name HE2 ))
  3.500 3.100 2.000 peak 10531 weight 0.10000E+01 volume 0.13341E+01 ppm1 7.613 ppm2 -0.480
ASSI {10541}
  (( segid "PROT" and resid 92 and name HN ))
  (( segid "PROT" and resid 92 and name HA ))
  3.500 3.100 2.000 peak 10541 weight 0.10000E+01 volume 0.12495E+01 ppm1 8.471 ppm2 4.224
ASSI {10551}
  (( segid "PROT" and resid 92 and name HN ))
  (( segid "PROT" and resid 90 and name HD1 ))
  3.100 2.400 2.400 peak 10551 weight 0.10000E+01 volume 0.27898E+01 ppm1 8.475 ppm2 4.115
ASSI {10561}
  (( segid "PROT" and resid 47 and name HN ))
  (( segid "PROT" and resid 47 and name HB1 ))
  3.200 2.600 2.300 peak 10561 weight 0.10000E+01 volume 0.23977E+01 ppm1 8.473 ppm2 3.212
ASSI {10571}
  (( segid "PROT" and resid 92 and name HN ))
  (( segid "PROT" and resid 92 and name HG1 ))
  3.200 2.600 2.300 peak 10571 weight 0.10000E+01 volume 0.22443E+01 ppm1 8.476 ppm2 2.389
ASSI {10581}
  (( segid "PROT" and resid 47 and name HN ))
  (( segid "PROT" and resid 46 and name HN ))
  3.100 2.400 2.400 peak 10581 weight 0.10000E+01 volume 0.29705E+01 ppm1 8.469 ppm2 8.038
ASSI {10601}
  (( segid "PROT" and resid 92 and name HN ))
  (( segid "PROT" and resid 96 and name HN ))
  3.400 2.900 2.100 peak 10601 weight 0.10000E+01 volume 0.16185E+01 ppm1 8.470 ppm2 7.383
ASSI {10621}
  (( segid "PROT" and resid 47 and name HN ))
  (( segid "PROT" and resid 47 and name HB2 ))
  3.000 2.200 2.200 peak 10621 weight 0.10000E+01 volume 0.34111E+01 ppm1 8.468 ppm2 2.819
ASSI {10631}
  (( segid "PROT" and resid 34 and name HN ))
  (( segid "PROT" and resid 33 and name HA ))
  3.300 2.700 2.200 peak 10631 weight 0.10000E+01 volume 0.18895E+01 ppm1 7.619 ppm2 3.944
ASSI {10641}
  (( segid "PROT" and resid 65 and name HD21 ))
  (( segid "PROT" and resid 65 and name HB2 ))
  3.200 2.600 2.300 peak 10641 weight 0.10000E+01 volume 0.22232E+01 ppm1 7.608 ppm2 2.798
ASSI {10651}
  (( segid "PROT" and resid 34 and name HN ))
  (( segid "PROT" and resid 56 and name HB1 ))
  3.400 2.900 2.100 peak 10651 weight 0.10000E+01 volume 0.16335E+01 ppm1 7.613 ppm2 2.105
ASSI {10661}
  (( segid "PROT" and resid 65 and name HD21 ))
  (( segid "PROT" and resid 65 and name HD22 ))
  2.200 1.200 1.200 peak 10661 weight 0.10000E+01 volume 0.19920E+02 ppm1 7.602 ppm2 6.975
ASSI {10671}
  (( segid "PROT" and resid 65 and name HD21 ))
  (( segid "PROT" and resid 65 and name HB1 ))
  3.400 2.900 2.100 peak 10671 weight 0.10000E+01 volume 0.16947E+01 ppm1 7.608 ppm2 3.037
ASSI {10691}
  (( segid "PROT" and resid 65 and name HD22 ))
  (( segid "PROT" and resid 65 and name HB1 ))
  3.500 3.100 2.000 peak 10691 weight 0.10000E+01 volume 0.13236E+01 ppm1 6.963 ppm2 3.024
ASSI {10701}
  (( segid "PROT" and resid 32 and name HE1 ))
  (( segid "PROT" and resid 32 and name HD1 ))
  2.600 1.700 1.700 peak 10701 weight 0.10000E+01 volume 0.72566E+01 ppm1 10.416 ppm2 7.865
ASSI {10731}
  (( segid "PROT" and resid 32 and name HE1 ))
  (( segid "PROT" and resid 30 and name HA ))
  3.200 2.600 2.300 peak 10731 weight 0.10000E+01 volume 0.23935E+01 ppm1 10.418 ppm2 4.831
ASSI {10741}
  (( segid "PROT" and resid 32 and name HE1 ))
  (( segid "PROT" and resid 32 and name HB2 ))
  3.500 3.100 2.000 peak 10741 weight 0.10000E+01 volume 0.12701E+01 ppm1 10.417 ppm2 3.361
ASSI {10771}
  (( segid "PROT" and resid 32 and name HE1 ))
  (( segid "PROT" and resid 32 and name HE3 ))
  3.100 2.400 2.400 peak 10771 weight 0.10000E+01 volume 0.27416E+01 ppm1 10.414 ppm2 7.340
ASSI {10791}

```

```

(( segid "PROT" and resid 32 and name HE1 ))
(( segid "PROT" and resid 29 and name HG2 ))
3.400 2.900 2.100 peak 10791 weight 0.10000E+01 volume 0.16873E+01 ppm1 10.419 ppm2 2.423
ASSI {10801}
(( segid "PROT" and resid 16 and name HN ))
(( segid "PROT" and resid 15 and name HD% ))
3.200 2.600 2.300 peak 10801 weight 0.10000E+01 volume 0.22526E+01 ppm1 8.194 ppm2 7.068
ASSI {10821}
(( segid "PROT" and resid 16 and name HN ))
(( segid "PROT" and resid 15 and name HN ))
2.600 1.700 1.700 peak 10821 weight 0.10000E+01 volume 0.86346E+01 ppm1 8.190 ppm2 7.998
ASSI {10851}
(( segid "PROT" and resid 16 and name HN ))
(( segid "PROT" and resid 12 and name HA ))
2.700 1.800 1.800 peak 10851 weight 0.10000E+01 volume 0.66059E+01 ppm1 8.188 ppm2 4.738
ASSI {10861}
(( segid "PROT" and resid 16 and name HN ))
(( segid "PROT" and resid 16 and name HA ))
2.900 2.100 2.100 peak 10861 weight 0.10000E+01 volume 0.42394E+01 ppm1 8.186 ppm2 4.176
ASSI {10871}
(( segid "PROT" and resid 16 and name HN ))
(( segid "PROT" and resid 16 and name HB1 ))
2.300 1.300 1.300 peak 10871 weight 0.10000E+01 volume 0.15224E+02 ppm1 8.189 ppm2 4.023
ASSI {10881}
(( segid "PROT" and resid 16 and name HN ))
(( segid "PROT" and resid 16 and name HB2 ))
2.500 1.600 1.600 peak 10881 weight 0.10000E+01 volume 0.91687E+01 ppm1 8.190 ppm2 3.935
ASSI {10891}
(( segid "PROT" and resid 16 and name HN ))
(( segid "PROT" and resid 15 and name HB1 ))
2.900 2.100 2.100 peak 10891 weight 0.10000E+01 volume 0.40710E+01 ppm1 8.189 ppm2 3.220
ASSI {10901}
(( segid "PROT" and resid 16 and name HN ))
(( segid "PROT" and resid 15 and name HB2 ))
2.700 1.800 1.800 peak 10901 weight 0.10000E+01 volume 0.61026E+01 ppm1 8.190 ppm2 3.051
ASSI {10911}
(( segid "PROT" and resid 16 and name HN ))
(( segid "PROT" and resid 18 and name HG ))
3.600 3.200 1.900 peak 10911 weight 0.10000E+01 volume 0.12027E+01 ppm1 8.188 ppm2 1.683
ASSI {10931}
(( segid "PROT" and resid 16 and name HN ))
(( segid "PROT" and resid 17 and name HB ))
3.400 2.900 2.100 peak 10931 weight 0.10000E+01 volume 0.16655E+01 ppm1 8.186 ppm2 4.263
ASSI {10951}
(( segid "PROT" and resid 29 and name HE21 ))
(( segid "PROT" and resid 29 and name HE22 ))
2.000 1.000 1.000 peak 10951 weight 0.10000E+01 volume 0.39167E+02 ppm1 7.574 ppm2 6.873
ASSI {11041}
(( segid "PROT" and resid 70 and name HN ))
(( segid "PROT" and resid 69 and name HN ))
2.500 1.600 1.600 peak 11041 weight 0.10000E+01 volume 0.10515E+02 ppm1 7.446 ppm2 7.703
ASSI {11051}
(( segid "PROT" and resid 70 and name HN ))
(( segid "PROT" and resid 68 and name HD% ))
3.400 2.900 2.100 peak 11051 weight 0.10000E+01 volume 0.15733E+01 ppm1 7.448 ppm2 7.174
ASSI {11061}
(( segid "PROT" and resid 70 and name HN ))
(( segid "PROT" and resid 74 and name HN ))
3.500 3.100 2.000 peak 11061 weight 0.10000E+01 volume 0.14404E+01 ppm1 7.452 ppm2 6.918
ASSI {11071}
(( segid "PROT" and resid 70 and name HN ))
(( segid "PROT" and resid 68 and name HA ))
2.900 2.100 2.100 peak 11071 weight 0.10000E+01 volume 0.37994E+01 ppm1 7.449 ppm2 4.548
ASSI {11081}
(( segid "PROT" and resid 70 and name HN ))
(( segid "PROT" and resid 70 and name HB1 ))
3.000 2.200 2.200 peak 11081 weight 0.10000E+01 volume 0.32723E+01 ppm1 7.445 ppm2 4.226
ASSI {11091}
(( segid "PROT" and resid 70 and name HN ))
(( segid "PROT" and resid 70 and name HB2 ))
3.000 2.200 2.200 peak 11091 weight 0.10000E+01 volume 0.35063E+01 ppm1 7.446 ppm2 3.774
ASSI {11101}
(( segid "PROT" and resid 70 and name HN ))
(( segid "PROT" and resid 68 and name HB2 ))
3.400 2.900 2.100 peak 11101 weight 0.10000E+01 volume 0.16583E+01 ppm1 7.446 ppm2 2.935
ASSI {11111}
(( segid "PROT" and resid 70 and name HN ))
(( segid "PROT" and resid 73 and name HB1 ))
3.100 2.400 2.400 peak 11111 weight 0.10000E+01 volume 0.29172E+01 ppm1 7.446 ppm2 2.000
ASSI {11121}
(( segid "PROT" and resid 70 and name HN ))
(( segid "PROT" and resid 73 and name HB2 ))
3.100 2.400 2.400 peak 11121 weight 0.10000E+01 volume 0.26620E+01 ppm1 7.447 ppm2 1.894
ASSI {11131}
(( segid "PROT" and resid 70 and name HN ))
(( segid "PROT" and resid 14 and name HD2% ))
2.500 1.600 1.600 peak 11131 weight 0.10000E+01 volume 0.11170E+02 ppm1 7.446 ppm2 0.836
ASSI {11141}
(( segid "PROT" and resid 70 and name HN ))

```

```

(( segid "PROT" and resid 69 and name HA ))
2.900 2.100 2.100 peak 11141 weight 0.10000E+01 volume 0.44901E+01 ppm1 7.445 ppm2 4.097
ASSI {11151}
(( segid "PROT" and resid 70 and name HN ))
(( segid "PROT" and resid 69 and name HB ))
3.200 2.600 2.300 peak 11151 weight 0.10000E+01 volume 0.25399E+01 ppm1 7.445 ppm2 2.326
ASSI {11161}
(( segid "PROT" and resid 70 and name HN ))
(( segid "PROT" and resid 73 and name HG ))
3.400 2.900 2.100 peak 11161 weight 0.10000E+01 volume 0.15757E+01 ppm1 7.443 ppm2 1.769
ASSI {11171}
(( segid "PROT" and resid 70 and name HN ))
(( segid "PROT" and resid 73 and name HD1% ))
2.500 1.600 1.600 peak 11171 weight 0.10000E+01 volume 0.10896E+02 ppm1 7.445 ppm2 0.952
ASSI {11181}
(( segid "PROT" and resid 79 and name HE21 ))
(( segid "PROT" and resid 79 and name HE22 ))
2.100 1.100 1.100 peak 11181 weight 0.10000E+01 volume 0.30858E+02 ppm1 7.315 ppm2 7.232
ASSI {11191}
(( segid "PROT" and resid 79 and name HE21 ))
(( segid "PROT" and resid 79 and name HG1 ))
3.000 2.200 2.200 peak 11191 weight 0.10000E+01 volume 0.31916E+01 ppm1 7.310 ppm2 2.457
ASSI {11221}
(( segid "PROT" and resid 79 and name HE22 ))
(( segid "PROT" and resid 79 and name HG1 ))
3.500 3.100 2.000 peak 11221 weight 0.10000E+01 volume 0.13222E+01 ppm1 7.232 ppm2 2.458
ASSI {11231}
(( segid "PROT" and resid 27 and name HN ))
(( segid "PROT" and resid 26 and name HN ))
2.600 1.700 1.700 peak 11231 weight 0.10000E+01 volume 0.89340E+01 ppm1 7.552 ppm2 8.572
ASSI {11241}
(( segid "PROT" and resid 27 and name HN ))
(( segid "PROT" and resid 27 and name HA ))
2.700 1.800 1.800 peak 11241 weight 0.10000E+01 volume 0.63843E+01 ppm1 7.552 ppm2 4.465
ASSI {11251}
(( segid "PROT" and resid 27 and name HN ))
(( segid "PROT" and resid 24 and name HA ))
3.000 2.200 2.200 peak 11251 weight 0.10000E+01 volume 0.31959E+01 ppm1 7.551 ppm2 4.188
ASSI {11261}
(( segid "PROT" and resid 27 and name HN ))
(( segid "PROT" and resid 28 and name HB1 ))
3.500 3.100 2.000 peak 11261 weight 0.10000E+01 volume 0.14785E+01 ppm1 7.552 ppm2 2.997
ASSI {11271}
(( segid "PROT" and resid 27 and name HN ))
(( segid "PROT" and resid 28 and name HB2 ))
3.500 3.100 2.000 peak 11271 weight 0.10000E+01 volume 0.13992E+01 ppm1 7.554 ppm2 2.778
ASSI {11291}
(( segid "PROT" and resid 27 and name HN ))
(( segid "PROT" and resid 31 and name HB% ))
3.400 2.900 2.100 peak 11291 weight 0.10000E+01 volume 0.14984E+01 ppm1 7.553 ppm2 1.733
ASSI {11301}
(( segid "PROT" and resid 27 and name HN ))
(( segid "PROT" and resid 27 and name HB1 ))
2.400 1.400 1.400 peak 11301 weight 0.10000E+01 volume 0.12213E+02 ppm1 7.551 ppm2 4.034
ASSI {11311}
(( segid "PROT" and resid 27 and name HN ))
(( segid "PROT" and resid 26 and name HA ))
2.900 2.100 2.100 peak 11311 weight 0.10000E+01 volume 0.39762E+01 ppm1 7.550 ppm2 3.908
ASSI {11321}
(( segid "PROT" and resid 27 and name HN ))
(( segid "PROT" and resid 26 and name HB1 ))
2.800 2.000 2.000 peak 11321 weight 0.10000E+01 volume 0.48756E+01 ppm1 7.551 ppm2 1.892
ASSI {11331}
(( segid "PROT" and resid 24 and name HE21 ))
(( segid "PROT" and resid 24 and name HE22 ))
2.100 1.100 1.100 peak 11331 weight 0.10000E+01 volume 0.25925E+02 ppm1 7.026 ppm2 6.911
ASSI {11341}
(( segid "PROT" and resid 24 and name HE21 ))
(( segid "PROT" and resid 24 and name HG1 ))
3.200 2.600 2.300 peak 11341 weight 0.10000E+01 volume 0.24518E+01 ppm1 7.025 ppm2 2.863
ASSI {11351}
(( segid "PROT" and resid 24 and name HE21 ))
(( segid "PROT" and resid 24 and name HG2 ))
3.400 2.900 2.100 peak 11351 weight 0.10000E+01 volume 0.16618E+01 ppm1 7.026 ppm2 2.481
ASSI {11371}
(( segid "PROT" and resid 24 and name HE22 ))
(( segid "PROT" and resid 24 and name HG1 ))
3.600 3.200 1.900 peak 11371 weight 0.10000E+01 volume 0.11102E+01 ppm1 6.903 ppm2 2.863
ASSI {11381}
(( segid "PROT" and resid 39 and name HN ))
(( segid "PROT" and resid 39 and name HG2 ))
3.000 2.200 2.200 peak 11381 weight 0.10000E+01 volume 0.31902E+01 ppm1 9.090 ppm2 1.449
ASSI {11391}
(( segid "PROT" and resid 39 and name HN ))
(( segid "PROT" and resid 38 and name HN ))
3.600 3.200 1.900 peak 11391 weight 0.10000E+01 volume 0.11942E+01 ppm1 9.087 ppm2 8.338
ASSI {11401}
(( segid "PROT" and resid 39 and name HN ))
(( segid "PROT" and resid 39 and name HA ))

```

3.100	2.400	2.400	peak 11401	weight 0.10000E+01	volume 0.26384E+01	ppm1 9.083	ppm2 4.436	
ASSI {11411}								
((segid "PROT" and resid 39 and name HN))								
((segid "PROT" and resid 38 and name HA))								
2.300	1.300	1.300	peak 11411	weight 0.10000E+01	volume 0.15682E+02	ppm1 9.086	ppm2 3.475	
ASSI {11431}								
((segid "PROT" and resid 39 and name HN))								
((segid "PROT" and resid 39 and name HB1))								
3.300	2.700	2.200	peak 11431	weight 0.10000E+01	volume 0.18750E+01	ppm1 9.085	ppm2 2.033	
ASSI {11441}								
((segid "PROT" and resid 39 and name HN))								
((segid "PROT" and resid 39 and name HB2))								
3.000	2.200	2.200	peak 11441	weight 0.10000E+01	volume 0.37080E+01	ppm1 9.083	ppm2 1.911	
ASSI {11451}								
((segid "PROT" and resid 39 and name HN))								
((segid "PROT" and resid 39 and name HD2))								
2.500	1.600	1.600	peak 11451	weight 0.10000E+01	volume 0.93310E+01	ppm1 9.086	ppm2 1.639	
ASSI {11461}								
((segid "PROT" and resid 39 and name HN))								
((segid "PROT" and resid 38 and name HB))								
3.500	3.100	2.000	peak 11461	weight 0.10000E+01	volume 0.12532E+01	ppm1 9.086	ppm2 1.057	
ASSI {11471}								
((segid "PROT" and resid 39 and name HN))								
((segid "PROT" and resid 38 and name HG1%))								
3.100	2.400	2.400	peak 11471	weight 0.10000E+01	volume 0.26696E+01	ppm1 9.082	ppm2 0.470	
ASSI {11481}								
((segid "PROT" and resid 39 and name HN))								
((segid "PROT" and resid 38 and name HG2%))								
2.800	2.000	2.000	peak 11481	weight 0.10000E+01	volume 0.55974E+01	ppm1 9.085	ppm2 -0.027	
ASSI {11491}								
((segid "PROT" and resid 76 and name HN))								
((segid "PROT" and resid 78 and name HN))								
2.600	1.700	1.700	peak 11491	weight 0.10000E+01	volume 0.88670E+01	ppm1 8.020	ppm2 7.383	
ASSI {11511}								
((segid "PROT" and resid 110 and name HN))								
((segid "PROT" and resid 111 and name HB1))								
3.400	2.900	2.100	peak 11511	weight 0.10000E+01	volume 0.16849E+01	ppm1 8.123	ppm2 1.889	
ASSI {11531}								
((segid "PROT" and resid 31 and name HN))								
((segid "PROT" and resid 29 and name HA))								
3.100	2.400	2.400	peak 11531	weight 0.10000E+01	volume 0.30332E+01	ppm1 7.915	ppm2 4.219	
ASSI {11541}								
((segid "PROT" and resid 31 and name HN))								
((segid "PROT" and resid 98 and name HB1))								
3.500	3.100	2.000	peak 11541	weight 0.10000E+01	volume 0.14720E+01	ppm1 7.918	ppm2 3.384	
ASSI {11551}								
((segid "PROT" and resid 31 and name HN))								
((segid "PROT" and resid 30 and name HB2))								
3.300	2.700	2.200	peak 11551	weight 0.10000E+01	volume 0.20522E+01	ppm1 7.914	ppm2 3.975	
ASSI {11561}								
((segid "PROT" and resid 87 and name HN))								
((segid "PROT" and resid 87 and name HB2))								
2.600	1.700	1.700	peak 11561	weight 0.10000E+01	volume 0.79508E+01	ppm1 7.951	ppm2 2.048	
ASSI {11571}								
((segid "PROT" and resid 75 and name HN))								
((segid "PROT" and resid 77 and name HN))								
3.400	2.900	2.100	peak 11571	weight 0.10000E+01	volume 0.16867E+01	ppm1 8.505	ppm2 7.389	
ASSI {11581}								
((segid "PROT" and resid 12 and name HN))								
((segid "PROT" and resid 15 and name HB1))								
3.600	3.200	1.900	peak 11581	weight 0.10000E+01	volume 0.10787E+01	ppm1 8.421	ppm2 3.231	
ASSI {11591}								
((segid "PROT" and resid 112 and name HN))								
((segid "PROT" and resid 110 and name HA))								
3.400	2.900	2.100	peak 11591	weight 0.10000E+01	volume 0.17506E+01	ppm1 8.062	ppm2 3.881	
ASSI {11611}								
((segid "PROT" and resid 9 and name HN))								
((segid "PROT" and resid 9 and name HB2))								
2.900	2.100	2.100	peak 11611	weight 0.10000E+01	volume 0.44369E+01	ppm1 8.447	ppm2 1.837	
ASSI {11621}								
((segid "PROT" and resid 63 and name HN))								
((segid "PROT" and resid 63 and name HA))								
3.000	2.200	2.200	peak 11621	weight 0.10000E+01	volume 0.36776E+01	ppm1 8.888	ppm2 4.695	
ASSI {11631}								
((segid "PROT" and resid 55 and name HN))								
((segid "PROT" and resid 56 and name HA))								
3.000	2.200	2.200	peak 11631	weight 0.10000E+01	volume 0.35373E+01	ppm1 7.381	ppm2 4.088	
ASSI {11641}								
((segid "PROT" and resid 55 and name HN))								
((segid "PROT" and resid 54 and name HE%))								
2.800	2.000	2.000	peak 11641	weight 0.10000E+01	volume 0.49789E+01	ppm1 7.384	ppm2 1.984	
ASSI {11651}								
((segid "PROT" and resid 55 and name HN))								
((segid "PROT" and resid 59 and name HB2))								
2.900	2.100	2.100	peak 11651	weight 0.10000E+01	volume 0.46532E+01	ppm1 7.383	ppm2 1.876	
ASSI {11661}								
((segid "PROT" and resid 27 and name HN))								
((segid "PROT" and resid 25 and name HG2%))								
3.600	3.200	1.900	peak 11661	weight 0.10000E+01	volume 0.11987E+01	ppm1 7.554	ppm2 1.036	


```

ASSI {11681}
(( segid "PROT" and resid 94 and name HN ))
(( segid "PROT" and resid 97 and name HG2 ))
2.900 2.100 2.100 peak 11681 weight 0.10000E+01 volume 0.38242E+01 ppm1 8.402 ppm2 1.585
ASSI {11691}
(( segid "PROT" and resid 24 and name HN ))
(( segid "PROT" and resid 23 and name HA ))
3.000 2.200 2.200 peak 11691 weight 0.10000E+01 volume 0.35931E+01 ppm1 8.042 ppm2 4.044
ASSI {11701}
(( segid "PROT" and resid 15 and name HN ))
(( segid "PROT" and resid 13 and name HA ))
3.200 2.600 2.300 peak 11701 weight 0.10000E+01 volume 0.21533E+01 ppm1 7.997 ppm2 4.181
ASSI {11711}
(( segid "PROT" and resid 29 and name HN ))
(( segid "PROT" and resid 31 and name HN ))
3.700 3.400 1.800 peak 11711 weight 0.10000E+01 volume 0.91890E+00 ppm1 8.580 ppm2 7.899
ASSI {11731}
(( segid "PROT" and resid 82 and name HN ))
(( segid "PROT" and resid 80 and name HA ))
3.700 3.400 1.800 peak 11731 weight 0.10000E+01 volume 0.10073E+01 ppm1 6.398 ppm2 4.050
ASSI {11741}
(( segid "PROT" and resid 82 and name HN ))
(( segid "PROT" and resid 78 and name HA ))
3.600 3.200 1.900 peak 11741 weight 0.10000E+01 volume 0.10688E+01 ppm1 6.397 ppm2 3.388
ASSI {11761}
(( segid "PROT" and resid 70 and name HN ))
(( segid "PROT" and resid 68 and name HB1 ))
3.700 3.400 1.800 peak 11761 weight 0.10000E+01 volume 0.91320E+00 ppm1 7.444 ppm2 3.074
ASSI {11781}
(( segid "PROT" and resid 32 and name HE1 ))
(( segid "PROT" and resid 32 and name HB1 ))
3.700 3.400 1.800 peak 11781 weight 0.10000E+01 volume 0.93370E+00 ppm1 10.419 ppm2 3.640
ASSI {11791}
(( segid "PROT" and resid 34 and name HN ))
(( segid "PROT" and resid 33 and name HG1 ))
3.700 3.400 1.800 peak 11791 weight 0.10000E+01 volume 0.92660E+00 ppm1 7.615 ppm2 0.252
ASSI {11801}
(( segid "PROT" and resid 34 and name HN ))
(( segid "PROT" and resid 102 and name HD18 ))
3.700 3.400 1.800 peak 11801 weight 0.10000E+01 volume 0.92480E+00 ppm1 7.614 ppm2 0.725
ASSI {11811}
(( segid "PROT" and resid 39 and name HN ))
(( segid "PROT" and resid 43 and name HN ))
3.700 3.400 1.800 peak 11811 weight 0.10000E+01 volume 0.96060E+00 ppm1 9.087 ppm2 7.184
ASSI {11851}
(( segid "PROT" and resid 27 and name HN ))
(( segid "PROT" and resid 25 and name HA ))
3.200 2.600 2.300 peak 11851 weight 0.10000E+01 volume 0.21545E+01 ppm1 7.551 ppm2 3.858
ASSI {11941}
(( segid "PROT" and resid 34 and name HN ))
(( segid "PROT" and resid 33 and name HG2 ))
3.800 3.600 1.700 peak 11941 weight 0.10000E+01 volume 0.80610E+00 ppm1 7.613 ppm2 -0.888
ASSI {11981}
(( segid "PROT" and resid 94 and name HN ))
(( segid "PROT" and resid 93 and name HA ))
3.700 3.400 1.800 peak 11981 weight 0.10000E+01 volume 0.93310E+00 ppm1 8.401 ppm2 4.504
ASSI {12011}
(( segid "PROT" and resid 94 and name HN ))
(( segid "PROT" and resid 95 and name HA ))
3.300 2.700 2.200 peak 12011 weight 0.10000E+01 volume 0.19064E+01 ppm1 8.402 ppm2 3.667
ASSI {12081}
(( segid "PROT" and resid 26 and name HN ))
(( segid "PROT" and resid 22 and name HA ))
3.400 2.900 2.100 peak 12081 weight 0.10000E+01 volume 0.15330E+01 ppm1 8.575 ppm2 4.116
ASSI {12101}
(( segid "PROT" and resid 68 and name HN ))
(( segid "PROT" and resid 63 and name HB1 ))
3.800 3.600 1.700 peak 12101 weight 0.10000E+01 volume 0.88970E+00 ppm1 8.010 ppm2 2.329
ASSI {12161}
(( segid "PROT" and resid 89 and name HN ))
(( segid "PROT" and resid 85 and name HA ))
3.600 3.200 1.900 peak 12161 weight 0.10000E+01 volume 0.10598E+01 ppm1 8.123 ppm2 4.469
ASSI {12201}
(( segid "PROT" and resid 108 and name HN ))
(( segid "PROT" and resid 110 and name HG11 ))
3.800 3.600 1.700 peak 12201 weight 0.10000E+01 volume 0.82640E+00 ppm1 7.931 ppm2 1.128
ASSI {12221}
(( segid "PROT" and resid 49 and name HN ))
(( segid "PROT" and resid 47 and name HB2 ))
3.700 3.400 1.800 peak 12221 weight 0.10000E+01 volume 0.10274E+01 ppm1 7.119 ppm2 2.796
ASSI {12231}
(( segid "PROT" and resid 49 and name HN ))
(( segid "PROT" and resid 48 and name HG1 ))
3.500 3.100 2.000 peak 12231 weight 0.10000E+01 volume 0.12697E+01 ppm1 7.117 ppm2 2.362
ASSI {12241}
(( segid "PROT" and resid 49 and name HN ))
(( segid "PROT" and resid 48 and name HG2 ))
3.600 3.200 1.900 peak 12241 weight 0.10000E+01 volume 0.11663E+01 ppm1 7.115 ppm2 2.243
ASSI {12251}

```

```

(( segid "PROT" and resid 49 and name HN ))
( segid "PROT" and resid 50 and name HG2%)
3.900 3.800 1.600 peak 12251 weight 0.10000E+01 volume 0.74400E+00 ppm1 7.114 ppm2 0.391
ASSI {12271}
(( segid "PROT" and resid 49 and name HN ))
(( segid "PROT" and resid 47 and name HN ))
3.700 3.400 1.800 peak 12271 weight 0.10000E+01 volume 0.10061E+01 ppm1 7.113 ppm2 8.447
ASSI {12281}
(( segid "PROT" and resid 83 and name HN ))
(( segid "PROT" and resid 85 and name HN ))
3.700 3.400 1.800 peak 12281 weight 0.10000E+01 volume 0.92080E+00 ppm1 9.095 ppm2 6.900
ASSI {12311}
(( segid "PROT" and resid 116 and name HN ))
( segid "PROT" and resid 110 and name HD1%)
3.600 3.200 1.900 peak 12311 weight 0.10000E+01 volume 0.11475E+01 ppm1 7.473 ppm2 0.537
ASSI {12421}
(( segid "PROT" and resid 75 and name HN ))
(( segid "PROT" and resid 78 and name HB2 ))
3.700 3.400 1.800 peak 12421 weight 0.10000E+01 volume 0.10440E+01 ppm1 8.512 ppm2 0.470
ASSI {12431}
(( segid "PROT" and resid 60 and name HN ))
(( segid "PROT" and resid 57 and name HN ))
3.800 3.600 1.700 peak 12431 weight 0.10000E+01 volume 0.87300E+00 ppm1 7.958 ppm2 8.813
ASSI {12461}
(( segid "PROT" and resid 60 and name HN ))
( segid "PROT" and resid 59 and name HE%)
3.700 3.400 1.800 peak 12461 weight 0.10000E+01 volume 0.95910E+00 ppm1 7.969 ppm2 1.273
ASSI {12501}
(( segid "PROT" and resid 82 and name HN ))
(( segid "PROT" and resid 79 and name HN ))
3.800 3.600 1.700 peak 12501 weight 0.10000E+01 volume 0.79110E+00 ppm1 6.397 ppm2 8.086
ASSI {12541}
(( segid "PROT" and resid 86 and name HN ))
(( segid "PROT" and resid 85 and name HA ))
3.700 3.400 1.800 peak 12541 weight 0.10000E+01 volume 0.10186E+01 ppm1 7.830 ppm2 4.477
ASSI {12551}
(( segid "PROT" and resid 86 and name HN ))
(( segid "PROT" and resid 84 and name HA ))
3.400 2.900 2.100 peak 12551 weight 0.10000E+01 volume 0.15928E+01 ppm1 7.829 ppm2 4.336
ASSI {12561}
(( segid "PROT" and resid 86 and name HN ))
(( segid "PROT" and resid 87 and name HB1 ))
3.700 3.400 1.800 peak 12561 weight 0.10000E+01 volume 0.10415E+01 ppm1 7.830 ppm2 2.209
ASSI {12621}
(( segid "PROT" and resid 85 and name HN ))
(( segid "PROT" and resid 83 and name HA ))
3.700 3.400 1.800 peak 12621 weight 0.10000E+01 volume 0.92730E+00 ppm1 6.910 ppm2 3.853
ASSI {12651}
(( segid "PROT" and resid 85 and name HN ))
(( segid "PROT" and resid 86 and name HG1 ))
3.800 3.600 1.700 peak 12651 weight 0.10000E+01 volume 0.89670E+00 ppm1 6.907 ppm2 1.311
ASSI {12661}
(( segid "PROT" and resid 85 and name HN ))
(( segid "PROT" and resid 86 and name HG2 ))
3.900 3.800 1.600 peak 12661 weight 0.10000E+01 volume 0.74160E+00 ppm1 6.911 ppm2 0.141
ASSI {12691}
(( segid "PROT" and resid 35 and name HN ))
(( segid "PROT" and resid 34 and name HB1 ))
3.500 3.100 2.000 peak 12691 weight 0.10000E+01 volume 0.12493E+01 ppm1 7.159 ppm2 3.483
ASSI {12711}
(( segid "PROT" and resid 97 and name HN ))
(( segid "PROT" and resid 93 and name HN ))
3.500 3.100 2.000 peak 12711 weight 0.10000E+01 volume 0.13450E+01 ppm1 7.960 ppm2 8.132
ASSI {12871}
(( segid "PROT" and resid 55 and name HN ))
(( segid "PROT" and resid 56 and name HN ))
3.700 3.400 1.800 peak 12871 weight 0.10000E+01 volume 0.94890E+00 ppm1 7.380 ppm2 9.125
ASSI {12891}
(( segid "PROT" and resid 54 and name HN ))
(( segid "PROT" and resid 55 and name HB1 ))
3.900 3.800 1.600 peak 12891 weight 0.10000E+01 volume 0.74390E+00 ppm1 8.519 ppm2 2.386
ASSI {12901}
(( segid "PROT" and resid 54 and name HN ))
( segid "PROT" and resid 81 and name HG1%)
3.600 3.200 1.900 peak 12901 weight 0.10000E+01 volume 0.10879E+01 ppm1 8.520 ppm2 0.484
ASSI {12911}
(( segid "PROT" and resid 89 and name HD21))
(( segid "PROT" and resid 89 and name HB1 ))
3.700 3.400 1.800 peak 12911 weight 0.10000E+01 volume 0.97110E+00 ppm1 8.352 ppm2 3.097
ASSI {12921}
(( segid "PROT" and resid 89 and name HD22))
(( segid "PROT" and resid 85 and name HB2 ))
3.700 3.400 1.800 peak 12921 weight 0.10000E+01 volume 0.98340E+00 ppm1 7.822 ppm2 3.091
ASSI {12981}
(( segid "PROT" and resid 77 and name HN ))
(( segid "PROT" and resid 79 and name HN ))
2.700 1.800 1.800 peak 12981 weight 0.10000E+01 volume 0.67122E+01 ppm1 7.380 ppm2 8.096
ASSI {13001}
(( segid "PROT" and resid 25 and name HN ))

```

```

(( segid "PROT" and resid 26 and name HB1 ))
3.600 3.200 1.900 peak 13001 weight 0.10000E+01 volume 0.11043E+01 ppm1 8.566 ppm2 1.896
ASSI {13071}
(( segid "PROT" and resid 22 and name HN ))
(( segid "PROT" and resid 20 and name HA ))
3.700 3.400 1.800 peak 13071 weight 0.10000E+01 volume 0.96300E+00 ppm1 8.853 ppm2 4.287
ASSI {13091}
(( segid "PROT" and resid 22 and name HN ))
(( segid "PROT" and resid 18 and name HA ))
3.700 3.400 1.800 peak 13091 weight 0.10000E+01 volume 0.91100E+00 ppm1 8.855 ppm2 3.287
ASSI {13111}
(( segid "PROT" and resid 22 and name HN ))
(( segid "PROT" and resid 18 and name HB1 ))
3.700 3.400 1.800 peak 13111 weight 0.10000E+01 volume 0.99160E+00 ppm1 8.855 ppm2 1.541
ASSI {13121}
(( segid "PROT" and resid 63 and name HN ))
(( segid "PROT" and resid 63 and name HD1*))
3.500 3.100 2.000 peak 13121 weight 0.10000E+01 volume 0.13848E+01 ppm1 8.853 ppm2 0.893
ASSI {13131}
(( segid "PROT" and resid 22 and name HN ))
(( segid "PROT" and resid 21 and name HD1*))
3.600 3.200 1.900 peak 13131 weight 0.10000E+01 volume 0.10970E+01 ppm1 8.855 ppm2 0.632
ASSI {13141}
(( segid "PROT" and resid 99 and name HN ))
(( segid "PROT" and resid 89 and name HD21))
3.700 3.400 1.800 peak 13141 weight 0.10000E+01 volume 0.98450E+00 ppm1 8.205 ppm2 8.372
ASSI {13161}
(( segid "PROT" and resid 99 and name HN ))
(( segid "PROT" and resid 96 and name HA ))
3.200 2.600 2.300 peak 13161 weight 0.10000E+01 volume 0.21348E+01 ppm1 8.192 ppm2 3.802
ASSI {13201}
(( segid "PROT" and resid 62 and name HN ))
(( segid "PROT" and resid 60 and name HB1 ))
3.700 3.400 1.800 peak 13201 weight 0.10000E+01 volume 0.10256E+01 ppm1 8.378 ppm2 4.220
ASSI {13221}
(( segid "PROT" and resid 64 and name HN ))
(( segid "PROT" and resid 63 and name HB2 ))
2.800 2.000 2.000 peak 13221 weight 0.10000E+01 volume 0.54381E+01 ppm1 8.023 ppm2 1.952
ASSI {13231}
(( segid "PROT" and resid 84 and name HN ))
(( segid "PROT" and resid 81 and name HN ))
3.800 3.600 1.700 peak 13231 weight 0.10000E+01 volume 0.82060E+00 ppm1 8.891 ppm2 7.048
ASSI {13241}
(( segid "PROT" and resid 17 and name HN ))
(( segid "PROT" and resid 19 and name HN ))
3.200 2.600 2.300 peak 13241 weight 0.10000E+01 volume 0.23334E+01 ppm1 8.069 ppm2 8.547
ASSI {13321}
(( segid "PROT" and resid 84 and name HN ))
(( segid "PROT" and resid 87 and name HN ))
3.600 3.200 1.900 peak 13321 weight 0.10000E+01 volume 0.11311E+01 ppm1 8.875 ppm2 7.947
ASSI {13331}
(( segid "PROT" and resid 84 and name HN ))
(( segid "PROT" and resid 86 and name HN ))
3.600 3.200 1.900 peak 13331 weight 0.10000E+01 volume 0.10625E+01 ppm1 8.875 ppm2 7.838
ASSI {13341}
(( segid "PROT" and resid 63 and name HN ))
(( segid "PROT" and resid 60 and name HA ))
3.600 3.200 1.900 peak 13341 weight 0.10000E+01 volume 0.12154E+01 ppm1 8.874 ppm2 4.429
ASSI {13351}
(( segid "PROT" and resid 106 and name HN ))
(( segid "PROT" and resid 107 and name HA ))
3.800 3.600 1.700 peak 13351 weight 0.10000E+01 volume 0.83500E+00 ppm1 9.148 ppm2 3.844
ASSI {13361}
(( segid "PROT" and resid 84 and name HN ))
(( segid "PROT" and resid 80 and name HD2 ))
3.800 3.600 1.700 peak 13361 weight 0.10000E+01 volume 0.82650E+00 ppm1 8.876 ppm2 3.295
ASSI {13421}
(( segid "PROT" and resid 9 and name HN ))
(( segid "PROT" and resid 9 and name HD1 ))
3.700 3.400 1.800 peak 13421 weight 0.10000E+01 volume 0.90930E+00 ppm1 8.449 ppm2 3.211
ASSI {13431}
(( segid "PROT" and resid 112 and name HN ))
(( segid "PROT" and resid 111 and name HG2 ))
3.200 2.600 2.300 peak 13431 weight 0.10000E+01 volume 0.24687E+01 ppm1 8.062 ppm2 1.315
ASSI {13471}
(( segid "PROT" and resid 43 and name HN ))
(( segid "PROT" and resid 42 and name HG1 ))
3.700 3.400 1.800 peak 13471 weight 0.10000E+01 volume 0.10242E+01 ppm1 7.179 ppm2 2.353
ASSI {13481}
(( segid "PROT" and resid 58 and name HN ))
(( segid "PROT" and resid 56 and name HN ))
3.700 3.400 1.800 peak 13481 weight 0.10000E+01 volume 0.91120E+00 ppm1 9.443 ppm2 9.140
ASSI {13521}
(( segid "PROT" and resid 10 and name HN ))
(( segid "PROT" and resid 13 and name HG1 ))
3.900 3.800 1.600 peak 13521 weight 0.10000E+01 volume 0.74580E+00 ppm1 8.303 ppm2 2.503
ASSI {13531}
(( segid "PROT" and resid 111 and name HN ))
(( segid "PROT" and resid 115 and name HN ))

```



```

ASSI { 2921}
  (( segid "PROT" and resid 18 and name HN ))
  ( segid "PROT" and resid 63 and name HD2%)
  3.400 2.900 2.100 peak 2921 weight 0.10000E+01 volume 0.17279E+01 ppm1 8.475 ppm2 1.048
ASSI { 3251}
  (( segid "PROT" and resid 17 and name HN ))
  ( segid "PROT" and resid 14 and name HD2%)
  3.400 2.900 2.100 peak 3251 weight 0.10000E+01 volume 0.16389E+01 ppm1 8.071 ppm2 0.805
OR { 3251}
  (( segid "PROT" and resid 17 and name HN ))
  ( segid "PROT" and resid 14 and name HD1%)
ASSI { 3281}
  (( segid "PROT" and resid 21 and name HN ))
  (( segid "PROT" and resid 24 and name HE21))
  3.500 3.100 2.000 peak 3281 weight 0.10000E+01 volume 0.14220E+01 ppm1 7 929 ppm2 7.046
ASSI { 3311}
  (( segid "PROT" and resid 21 and name HN ))
  ( segid "PROT" and resid 17 and name HG2%)
  3.200 2.600 2.300 peak 3311 weight 0.10000E+01 volume 0.21566E+01 ppm1 7.925 ppm2 1.144
ASSI { 3481}
  (( segid "PROT" and resid 64 and name HN ))
  (( segid "PROT" and resid 61 and name HB1 ))
  3.100 2.400 2.400 peak 3481 weight 0.10000E+01 volume 0.25719E+01 ppm1 8 025 ppm2 2.212
OR { 3481}
  (( segid "PROT" and resid 64 and name HN ))
  (( segid "PROT" and resid 61 and name HG2 ))
ASSI { 4021}
  (( segid "PROT" and resid 101 and name HN ))
  ( segid "PROT" and resid 99 and name HB%)
  3.000 2.200 2.200 peak 4021 weight 0.10000E+01 volume 0.33742E+01 ppm1 8.016 ppm2 1.608
ASSI { 4281}
  (( segid "PROT" and resid 101 and name HN ))
  (( segid "PROT" and resid 102 and name HB1 ))
  3.100 2.400 2.400 peak 4281 weight 0.10000E+01 volume 0.30641E+01 ppm1 8.020 ppm2 1.423
ASSI { 4481}
  (( segid "PROT" and resid 96 and name HN ))
  (( segid "PROT" and resid 90 and name HD2 ))
  3.100 2.400 2.400 peak 4481 weight 0.10000E+01 volume 0.28902E+01 ppm1 7.380 ppm2 3.918
ASSI { 4671}
  (( segid "PROT" and resid 30 and name HN ))
  ( segid "PROT" and resid 102 and name HD1%)
  3.400 2.900 2.100 peak 4671 weight 0.10000E+01 volume 0.15055E+01 ppm1 11.693 ppm2 0.737
OR { 4671}
  (( segid "PROT" and resid 30 and name HN ))
  ( segid "PROT" and resid 102 and name HD2%)
ASSI { 5721}
  (( segid "PROT" and resid 107 and name HN ))
  (( segid "PROT" and resid 24 and name HE21))
  3.200 2.600 2.300 peak 5721 weight 0.10000E+01 volume 0.22871E+01 ppm1 8.402 ppm2 7.065
ASSI { 6921}
  (( segid "PROT" and resid 85 and name HN ))
  (( segid "PROT" and resid 86 and name HB1 ))
  3.500 3.100 2.000 peak 6921 weight 0.10000E+01 volume 0.12926E+01 ppm1 6.894 ppm2 1.777
ASSI { 7091}
  (( segid "PROT" and resid 85 and name HN ))
  ( segid "PROT" and resid 99 and name HB%)
  3.400 2.900 2.100 peak 7091 weight 0.10000E+01 volume 0.15606E+01 ppm1 6.912 ppm2 1.640
ASSI { 7131}
  (( segid "PROT" and resid 23 and name HN ))
  ( segid "PROT" and resid 25 and name HG1%)
  3.600 3.200 1.900 peak 7131 weight 0.10000E+01 volume 0.11801E+01 ppm1 8.589 ppm2 1.237
ASSI { 7561}
  (( segid "PROT" and resid 82 and name HN ))
  (( segid "PROT" and resid 80 and name HB2 ))
  3.600 3.200 1.900 peak 7561 weight 0.10000E+01 volume 0.12116E+01 ppm1 6.400 ppm2 1.912
ASSI { 7821}
  (( segid "PROT" and resid 98 and name HN ))
  (( segid "PROT" and resid 34 and name HZ ))
  3.500 3.100 2.000 peak 7821 weight 0.10000E+01 volume 0.13298E+01 ppm1 8.471 ppm2 7.275
ASSI { 8461}
  (( segid "PROT" and resid 75 and name HN ))
  ( segid "PROT" and resid 76 and name HB%)
  3.200 2.600 2.300 peak 8461 weight 0.10000E+01 volume 0.21341E+01 ppm1 8.505 ppm2 1.518
ASSI { 9801}
  (( segid "PROT" and resid 68 and name HN ))
  (( segid "PROT" and resid 65 and name HB2 ))
  3.400 2.900 2.100 peak 9801 weight 0.10000E+01 volume 0.17553E+01 ppm1 7.992 ppm2 2.790
ASSI {10381}
  (( segid "PROT" and resid 20 and name HN ))
  ( segid "PROT" and resid 63 and name HD1%)
  3.400 2.900 2.100 peak 10381 weight 0.10000E+01 volume 0.17105E+01 ppm1 7.544 ppm2 0.890
ASSI {10511}
  (( segid "PROT" and resid 34 and name HN ))
  ( segid "PROT" and resid 56 and name HD1%)
  3.100 2.400 2.400 peak 10511 weight 0.10000E+01 volume 0.26440E+01 ppm1 7 610 ppm2 0.954
ASSI {11201}
  (( segid "PROT" and resid 79 and name HE21))
  (( segid "PROT" and resid 79 and name HB2 ))
  3.500 3.100 2.000 peak 11201 weight 0.10000E+01 volume 0.12542E+01 ppm1 7.314 ppm2 2.072

```

```

ASSI {11281}
(( segid "PROT" and resid 27 and name HN ))
(( segid "PROT" and resid 24 and name HB1 ))
3.600 3.200 1.900 peak 11281 weight 0.10000E+01 volume 0.11570E+01 ppm1 7.551 ppm2 2.509
OR {11281}
(( segid "PROT" and resid 27 and name HN ))
(( segid "PROT" and resid 24 and name HG2 ))
ASSI {11521}
(( segid "PROT" and resid 31 and name HN ))
(( segid "PROT" and resid 31 and name HA ))
3.400 2.900 2.100 peak 11521 weight 0.10000E+01 volume 0.15623E+01 ppm1 7.904 ppm2 4.412
ASSI {11891}
(( segid "PROT" and resid 70 and name HN ))
(( segid "PROT" and resid 18 and name HD1% ))
3.400 2.900 2.100 peak 11891 weight 0.10000E+01 volume 0.16604E+01 ppm1 7.447 ppm2 0.738
ASSI {11961}
(( segid "PROT" and resid 20 and name HN ))
(( segid "PROT" and resid 22 and name HB1 ))
3.800 3.600 1.700 peak 11961 weight 0.10000E+01 volume 0.79920E+00 ppm1 7.546 ppm2 2.090
ASSI {11971}
(( segid "PROT" and resid 94 and name HN ))
(( segid "PROT" and resid 90 and name HA ))
3.700 3.400 1.800 peak 11971 weight 0.10000E+01 volume 0.96270E+00 ppm1 8.401 ppm2 4.644
ASSI {12001}
(( segid "PROT" and resid 94 and name HN ))
(( segid "PROT" and resid 90 and name HD1 ))
3.600 3.200 1.900 peak 12001 weight 0.10000E+01 volume 0.11885E+01 ppm1 8.401 ppm2 4.108
ASSI {12051}
(( segid "PROT" and resid 79 and name HN ))
(( segid "PROT" and resid 75 and name HB1 ))
3.700 3.400 1.800 peak 12051 weight 0.10000E+01 volume 0.92950E+00 ppm1 8.100 ppm2 2.912
ASSI {12061}
(( segid "PROT" and resid 79 and name HN ))
(( segid "PROT" and resid 78 and name HD2% ))
3.700 3.400 1.800 peak 12061 weight 0.10000E+01 volume 0.93350E+00 ppm1 8.101 ppm2 0.165
ASSI {12141}
(( segid "PROT" and resid 89 and name HN ))
(( segid "PROT" and resid 96 and name HD% ))
3.700 3.400 1.800 peak 12141 weight 0.10000E+01 volume 0.10188E+01 ppm1 8.115 ppm2 7.097
ASSI {12151}
(( segid "PROT" and resid 89 and name HN ))
(( segid "PROT" and resid 95 and name HD% ))
3.800 3.600 1.700 peak 12151 weight 0.10000E+01 volume 0.83030E+00 ppm1 8.117 ppm2 6.849
ASSI {12181}
(( segid "PROT" and resid 89 and name HN ))
(( segid "PROT" and resid 90 and name HD1 ))
3.800 3.600 1.700 peak 12181 weight 0.10000E+01 volume 0.78650E+00 ppm1 8.115 ppm2 4.076
ASSI {12301}
(( segid "PROT" and resid 116 and name HN ))
(( segid "PROT" and resid 112 and name HN ))
3.700 3.400 1.800 peak 12301 weight 0.10000E+01 volume 0.10505E+01 ppm1 7.480 ppm2 8.064
ASSI {12341}
(( segid "PROT" and resid 69 and name HN ))
(( segid "PROT" and resid 68 and name HD% ))
3.700 3.400 1.800 peak 12341 weight 0.10000E+01 volume 0.10495E+01 ppm1 7.708 ppm2 7.143
ASSI {12391}
(( segid "PROT" and resid 56 and name HN ))
(( segid "PROT" and resid 34 and name HB2 ))
3.700 3.400 1.800 peak 12391 weight 0.10000E+01 volume 0.10296E+01 ppm1 9.134 ppm2 2.567
ASSI {12471}
(( segid "PROT" and resid 32 and name HN ))
(( segid "PROT" and resid 32 and name HE3 ))
3.700 3.400 1.800 peak 12471 weight 0.10000E+01 volume 0.94240E+00 ppm1 7.098 ppm2 7.314
ASSI {12481}
(( segid "PROT" and resid 32 and name HN ))
(( segid "PROT" and resid 34 and name HB2 ))
3.700 3.400 1.800 peak 12481 weight 0.10000E+01 volume 0.97880E+00 ppm1 7.103 ppm2 2.572
ASSI {12511}
(( segid "PROT" and resid 82 and name HN ))
(( segid "PROT" and resid 84 and name HB2 ))
3.900 3.800 1.600 peak 12511 weight 0.10000E+01 volume 0.71250E+00 ppm1 6.400 ppm2 2.689
ASSI {12581}
(( segid "PROT" and resid 86 and name HN ))
(( segid "PROT" and resid 87 and name HB2 ))
3.700 3.400 1.800 peak 12581 weight 0.10000E+01 volume 0.93270E+00 ppm1 7.832 ppm2 2.045
ASSI {12601}
(( segid "PROT" and resid 23 and name HN ))
(( segid "PROT" and resid 19 and name HB2 ))
3.700 3.400 1.800 peak 12601 weight 0.10000E+01 volume 0.90500E+00 ppm1 8.583 ppm2 1.394
ASSI {12631}
(( segid "PROT" and resid 85 and name HN ))
(( segid "PROT" and resid 87 and name HB1 ))
3.700 3.400 1.800 peak 12631 weight 0.10000E+01 volume 0.90190E+00 ppm1 6.908 ppm2 2.174
ASSI {12681}
(( segid "PROT" and resid 81 and name HN ))
(( segid "PROT" and resid 85 and name HN ))
3.500 3.100 2.000 peak 12681 weight 0.10000E+01 volume 0.13641E+01 ppm1 7.032 ppm2 6.863
ASSI {12721}
(( segid "PROT" and resid 97 and name HN ))

```

```

( segid "PROT" and resid 96 and name HD% )
3.600 3.200 1.900 peak 12721 weight 0.10000E+01 volume 0.11781E+01 ppm1 7.964 ppm2 7.096
ASSI {12751}
(( segid "PROT" and resid 107 and name HN ))
(( segid "PROT" and resid 108 and name HA ))
3.700 3.400 1.800 peak 12751 weight 0.10000E+01 volume 0.93010E+00 ppm1 8.399 ppm2 4.217
ASSI {12801}
(( segid "PROT" and resid 74 and name HN ))
(( segid "PROT" and resid 75 and name HG2 ))
3.600 3.200 1.900 peak 12801 weight 0.10000E+01 volume 0.10996E+01 ppm1 6.922 ppm2 2.202
ASSI {12811}
(( segid "PROT" and resid 74 and name HN ))
( segid "PROT" and resid 76 and name HB% )
3.700 3.400 1.800 peak 12811 weight 0.10000E+01 volume 0.93300E+00 ppm1 6.922 ppm2 1.505
ASSI {12831}
(( segid "PROT" and resid 30 and name HN ))
(( segid "PROT" and resid 32 and name HE3 ))
3.800 3.600 1.700 peak 12831 weight 0.10000E+01 volume 0.82040E+00 ppm1 11.693 ppm2 7.371
ASSI {12841}
(( segid "PROT" and resid 30 and name HN ))
(( segid "PROT" and resid 101 and name HB ))
3.800 3.600 1.700 peak 12841 weight 0.10000E+01 volume 0.82760E+00 ppm1 11.697 ppm2 1.892
ASSI {12991}
(( segid "PROT" and resid 96 and name HN ))
(( segid "PROT" and resid 89 and name HA ))
3.900 3.800 1.600 peak 12991 weight 0.10000E+01 volume 0.74480E+00 ppm1 7.378 ppm2 5.068
ASSI {13051}
(( segid "PROT" and resid 22 and name HN ))
(( segid "PROT" and resid 24 and name HE21 ))
3.400 2.900 2.100 peak 13051 weight 0.10000E+01 volume 0.17366E+01 ppm1 8.852 ppm2 7.062
ASSI {13261}
(( segid "PROT" and resid 17 and name HN ))
( segid "PROT" and resid 18 and name HD2% )
3.800 3.600 1.700 peak 13261 weight 0.10000E+01 volume 0.84610E+00 ppm1 8.070 ppm2 -0.192
ASSI {13301}
(( segid "PROT" and resid 21 and name HN ))
(( segid "PROT" and resid 22 and name HB1 ))
3.200 2.600 2.300 peak 13301 weight 0.10000E+01 volume 0.21404E+01 ppm1 7.927 ppm2 2.069
ASSI {13401}
(( segid "PROT" and resid 21 and name HN ))
( segid "PROT" and resid 24 and name HG1 ))
3.800 3.600 1.700 peak 13401 weight 0.10000E+01 volume 0.89640E+00 ppm1 7.957 ppm2 2.829
ASSI {13511}
(( segid "PROT" and resid 58 and name HN ))
(( segid "PROT" and resid 61 and name HG2 ))
2.900 2.100 2.100 peak 13511 weight 0.10000E+01 volume 0.44447E+01 ppm1 9.443 ppm2 2.259
OR {13511}
(( segid "PROT" and resid 58 and name HN ))
(( segid "PROT" and resid 61 and name HB1 ))
ASSI {13791}
(( segid "PROT" and resid 50 and name HN ))
(( segid "PROT" and resid 87 and name HB2 ))
3.800 3.600 1.700 peak 13791 weight 0.10000E+01 volume 0.77760E+00 ppm1 7.960 ppm2 2.038
ASSI {13931}
(( segid "PROT" and resid 115 and name HN ))
(( segid "PROT" and resid 111 and name HG2 ))
3.500 3.100 2.000 peak 13931 weight 0.10000E+01 volume 0.12820E+01 ppm1 7.749 ppm2 1.285
ASSI {14011}
(( segid "PROT" and resid 52 and name HN ))
( segid "PROT" and resid 50 and name HD1% )
3.600 3.200 1.900 peak 14011 weight 0.10000E+01 volume 0.12035E+01 ppm1 8.422 ppm2 0.549
ASSI {14041}
(( segid "PROT" and resid 99 and name HN ))
( segid "PROT" and resid 34 and name HE% )
3.500 3.100 2.000 peak 14041 weight 0.10000E+01 volume 0.14222E+01 ppm1 8.189 ppm2 7.221
ASSI { 12}
(( segid "PROT" and resid 17 and name HA ))
(( segid "PROT" and resid 17 and name HB ))
2.300 1.300 1.300 peak 12 weight 0.10000E+01 volume 0.64338E+01 ppm1 3.970 ppm2 4.285
ASSI { 42}
( segid "PROT" and resid 14 and name HD2% )
(( segid "PROT" and resid 17 and name HB ))
2.800 2.000 2.000 peak 42 weight 0.10000E+01 volume 0.23074E+01 ppm1 0.832 ppm2 4.289
ASSI { 72}
(( segid "PROT" and resid 58 and name HA ))
(( segid "PROT" and resid 58 and name HB ))
2.300 1.300 1.300 peak 72 weight 0.10000E+01 volume 0.68641E+01 ppm1 3.881 ppm2 4.117
ASSI { 92}
(( segid "PROT" and resid 25 and name HB ))
(( segid "PROT" and resid 25 and name HA ))
2.700 1.800 1.800 peak 92 weight 0.10000E+01 volume 0.23933E+01 ppm1 2.440 ppm2 3.873
ASSI { 102}
( segid "PROT" and resid 58 and name HG2% )
(( segid "PROT" and resid 58 and name HA ))
2.200 1.200 1.200 peak 102 weight 0.10000E+01 volume 0.90603E+01 ppm1 1.092 ppm2 3.879
ASSI { 122}
(( segid "PROT" and resid 20 and name HB1 ))
(( segid "PROT" and resid 17 and name HA ))
2.400 1.400 1.400 peak 122 weight 0.10000E+01 volume 0.59096E+01 ppm1 4 103 ppm2 3.964

```

```

ASSI { 132}
(( segid "PROT" and resid 61 and name HG2 ))
(( segid "PROT" and resid 58 and name HA ))
2.800 2.000 2.000 peak 132 weight 0.10000E+01 volume 0.23380E+01 ppm1 2.261 ppm2 3.883
ASSI { 142}
(( segid "PROT" and resid 17 and name HG2% ))
(( segid "PROT" and resid 17 and name HA ))
2.100 1.100 1.100 peak 142 weight 0.10000E+01 volume 0.10421E+02 ppm1 1.179 ppm2 3.970
ASSI { 172}
(( segid "PROT" and resid 83 and name HB ))
(( segid "PROT" and resid 83 and name HA ))
2.200 1.200 1.200 peak 172 weight 0.10000E+01 volume 0.96793E+01 ppm1 4.238 ppm2 3.876
ASSI { 182}
(( segid "PROT" and resid 86 and name HB1 ))
(( segid "PROT" and resid 83 and name HA ))
2.800 2.000 2.000 peak 182 weight 0.10000E+01 volume 0.23242E+01 ppm1 1.777 ppm2 3.898
ASSI { 232}
(( segid "PROT" and resid 70 and name HA ))
(( segid "PROT" and resid 70 and name HB1 ))
2.300 1.300 1.300 peak 232 weight 0.10000E+01 volume 0.74409E+01 ppm1 4.807 ppm2 4.232
ASSI { 242}
(( segid "PROT" and resid 70 and name HA ))
(( segid "PROT" and resid 70 and name HB2 ))
2.400 1.400 1.400 peak 242 weight 0.10000E+01 volume 0.57670E+01 ppm1 4.803 ppm2 3.793
ASSI { 252}
(( segid "PROT" and resid 70 and name HB1 ))
(( segid "PROT" and resid 70 and name HB2 ))
1.800 0.800 0.800 peak 252 weight 0.10000E+01 volume 0.26334E+02 ppm1 4.233 ppm2 3.789
ASSI { 272}
(( segid "PROT" and resid 69 and name HG2% ))
(( segid "PROT" and resid 70 and name HB2 ))
2.700 1.800 1.800 peak 272 weight 0.10000E+01 volume 0.27129E+01 ppm1 0.861 ppm2 3.787
ASSI { 292}
(( segid "PROT" and resid 30 and name HB1 ))
(( segid "PROT" and resid 98 and name HA ))
2.800 2.000 2.000 peak 292 weight 0.10000E+01 volume 0.21823E+01 ppm1 4.352 ppm2 4.223
ASSI { 302}
(( segid "PROT" and resid 98 and name HB1 ))
(( segid "PROT" and resid 98 and name HA ))
2.700 1.800 1.800 peak 302 weight 0.10000E+01 volume 0.24715E+01 ppm1 3.396 ppm2 4.223
ASSI { 342}
(( segid "PROT" and resid 11 and name HB1 ))
(( segid "PROT" and resid 11 and name HA ))
2.200 1.200 1.200 peak 342 weight 0.10000E+01 volume 0.86937E+01 ppm1 2.382 ppm2 4.376
ASSI { 362}
(( segid "PROT" and resid 101 and name HB ))
(( segid "PROT" and resid 101 and name HA ))
2.400 1.400 1.400 peak 362 weight 0.10000E+01 volume 0.53397E+01 ppm1 1.953 ppm2 3.694
ASSI { 372}
(( segid "PROT" and resid 101 and name HG11 ))
(( segid "PROT" and resid 101 and name HA ))
2.400 1.400 1.400 peak 372 weight 0.10000E+01 volume 0.50966E+01 ppm1 1.902 ppm2 3.693
ASSI { 382}
(( segid "PROT" and resid 14 and name HB1 ))
(( segid "PROT" and resid 11 and name HA ))
2.800 2.000 2.000 peak 382 weight 0.10000E+01 volume 0.20827E+01 ppm1 1.895 ppm2 4.377
ASSI { 392}
(( segid "PROT" and resid 101 and name HG12 ))
(( segid "PROT" and resid 101 and name HA ))
2.400 1.400 1.400 peak 392 weight 0.10000E+01 volume 0.47337E+01 ppm1 1.240 ppm2 3.693
ASSI { 402}
(( segid "PROT" and resid 101 and name HG2% ))
(( segid "PROT" and resid 101 and name HA ))
2.200 1.200 1.200 peak 402 weight 0.10000E+01 volume 0.91301E+01 ppm1 1.026 ppm2 3.696
ASSI { 422}
(( segid "PROT" and resid 33 and name HB2 ))
(( segid "PROT" and resid 33 and name HA ))
2.900 2.100 2.100 peak 422 weight 0.10000E+01 volume 0.17116E+01 ppm1 -0.429 ppm2 3.992
ASSI { 432}
(( segid "PROT" and resid 44 and name HB2 ))
(( segid "PROT" and resid 44 and name HA ))
2.600 1.700 1.700 peak 432 weight 0.10000E+01 volume 0.33766E+01 ppm1 2.059 ppm2 4.551
ASSI { 442}
(( segid "PROT" and resid 110 and name HB ))
(( segid "PROT" and resid 110 and name HA ))
2.300 1.300 1.300 peak 442 weight 0.10000E+01 volume 0.67160E+01 ppm1 1.794 ppm2 3.855
ASSI { 452}
(( segid "PROT" and resid 115 and name HB2 ))
(( segid "PROT" and resid 110 and name HA ))
2.700 1.800 1.800 peak 452 weight 0.10000E+01 volume 0.27910E+01 ppm1 1.609 ppm2 3.856
ASSI { 462}
(( segid "PROT" and resid 113 and name HB% ))
(( segid "PROT" and resid 110 and name HA ))
2.300 1.300 1.300 peak 462 weight 0.10000E+01 volume 0.65923E+01 ppm1 1.410 ppm2 3.857
ASSI { 472}
(( segid "PROT" and resid 17 and name HG2% ))
(( segid "PROT" and resid 110 and name HA ))
2.900 2.100 2.100 peak 472 weight 0.10000E+01 volume 0.18150E+01 ppm1 1.168 ppm2 3.856
ASSI { 492}

```



```

( segid "PROT" and resid 110 and name HD1%)
(( segid "PROT" and resid 110 and name HA ))
2.500 1.600 1.600 peak 492 weight 0.10000E+01 volume 0.43046E+01 ppm1 0.568 ppm2 3.857
ASSI { 502}
(( segid "PROT" and resid 27 and name HA ))
(( segid "PROT" and resid 27 and name HB1 ))
2.100 1.100 1.100 peak 502 weight 0.10000E+01 volume 0.13211E+02 ppm1 4.487 ppm2 4.051
ASSI { 522}
(( segid "PROT" and resid 5 and name HA ))
(( segid "PROT" and resid 5 and name HB2 ))
2.200 1.200 1.200 peak 522 weight 0.10000E+01 volume 0.86878E+01 ppm1 4.471 ppm2 3.905
ASSI { 542}
(( segid "PROT" and resid 38 and name HB ))
(( segid "PROT" and resid 38 and name HA ))
2.700 1.800 1.800 peak 542 weight 0.10000E+01 volume 0.26095E+01 ppm1 1.072 ppm2 3.492
ASSI { 552}
( segid "PROT" and resid 38 and name HG1%)
(( segid "PROT" and resid 38 and name HA ))
2.100 1.100 1.100 peak 552 weight 0.10000E+01 volume 0.10687E+02 ppm1 0.496 ppm2 3.493
ASSI { 572}
(( segid "PROT" and resid 30 and name HA ))
(( segid "PROT" and resid 30 and name HB2 ))
2.900 2.100 2.100 peak 572 weight 0.10000E+01 volume 0.17806E+01 ppm1 4.854 ppm2 3.992
ASSI { 582}
(( segid "PROT" and resid 30 and name HB2 ))
(( segid "PROT" and resid 30 and name HB1 ))
2.300 1.300 1.300 peak 582 weight 0.10000E+01 volume 0.65273E+01 ppm1 3.978 ppm2 4.346
ASSI { 632}
(( segid "PROT" and resid 37 and name HB1 ))
(( segid "PROT" and resid 37 and name HA ))
2.200 1.200 1.200 peak 632 weight 0.10000E+01 volume 0.90616E+01 ppm1 2.379 ppm2 4.272
ASSI { 642}
(( segid "PROT" and resid 8 and name HB1 ))
(( segid "PROT" and resid 8 and name HA ))
2.300 1.300 1.300 peak 642 weight 0.10000E+01 volume 0.70364E+01 ppm1 2.293 ppm2 4.460
ASSI { 662}
(( segid "PROT" and resid 37 and name HG1 ))
(( segid "PROT" and resid 37 and name HA ))
2.800 2.000 2.000 peak 662 weight 0.10000E+01 volume 0.21062E+01 ppm1 2.184 ppm2 4.272
ASSI { 682}
(( segid "PROT" and resid 49 and name HB ))
(( segid "PROT" and resid 49 and name HA ))
2.300 1.300 1.300 peak 682 weight 0.10000E+01 volume 0.72941E+01 ppm1 1.931 ppm2 4.111
ASSI { 702}
(( segid "PROT" and resid 37 and name HB2 ))
(( segid "PROT" and resid 37 and name HA ))
2.600 1.700 1.700 peak 702 weight 0.10000E+01 volume 0.31708E+01 ppm1 1.702 ppm2 4.271
ASSI { 712}
( segid "PROT" and resid 49 and name HG2%)
(( segid "PROT" and resid 49 and name HA ))
2.300 1.300 1.300 peak 712 weight 0.10000E+01 volume 0.71135E+01 ppm1 0.908 ppm2 4.109
ASSI { 742}
(( segid "PROT" and resid 60 and name HA ))
(( segid "PROT" and resid 60 and name HB1 ))
2.500 1.600 1.600 peak 742 weight 0.10000E+01 volume 0.38154E+01 ppm1 4.444 ppm2 4.248
ASSI { 752}
(( segid "PROT" and resid 60 and name HA ))
(( segid "PROT" and resid 60 and name HB2 ))
2.100 1.100 1.100 peak 752 weight 0.10000E+01 volume 0.11798E+02 ppm1 4.442 ppm2 4.065
ASSI { 762}
(( segid "PROT" and resid 41 and name HB ))
(( segid "PROT" and resid 41 and name HA ))
1.800 0.800 0.800 peak 762 weight 0.10000E+01 volume 0.34478E+02 ppm1 4.331 ppm2 4.095
ASSI { 772}
(( segid "PROT" and resid 46 and name HB1 ))
(( segid "PROT" and resid 46 and name HA ))
2.700 1.800 1.800 peak 772 weight 0.10000E+01 volume 0.24573E+01 ppm1 2.762 ppm2 3.505
ASSI { 782}
(( segid "PROT" and resid 46 and name HB2 ))
(( segid "PROT" and resid 46 and name HA ))
2.900 2.100 2.100 peak 782 weight 0.10000E+01 volume 0.16661E+01 ppm1 2.431 ppm2 3.504
ASSI { 842}
( segid "PROT" and resid 15 and name HD%)
(( segid "PROT" and resid 15 and name HA ))
2.800 2.000 2.000 peak 842 weight 0.10000E+01 volume 0.20619E+01 ppm1 7.104 ppm2 4.049
ASSI { 852}
(( segid "PROT" and resid 15 and name HB1 ))
(( segid "PROT" and resid 15 and name HA ))
2.500 1.600 1.600 peak 852 weight 0.10000E+01 volume 0.46305E+01 ppm1 3.250 ppm2 4.046
ASSI { 862}
(( segid "PROT" and resid 15 and name HB2 ))
(( segid "PROT" and resid 15 and name HA ))
2.600 1.700 1.700 peak 862 weight 0.10000E+01 volume 0.35482E+01 ppm1 3.085 ppm2 4.045
ASSI { 912}
( segid "PROT" and resid 69 and name HG2%)
(( segid "PROT" and resid 69 and name HA ))
2.300 1.300 1.300 peak 912 weight 0.10000E+01 volume 0.63782E+01 ppm1 0.861 ppm2 4.123
ASSI { 932}
(( segid "PROT" and resid 85 and name HB2 ))

```

```

(( segid "PROT" and resid 85 and name HA ))
2.800 2.000 2.000 peak 932 weight 0.10000E+01 volume 0.20935E+01 ppm1 3.093 ppm2 4.513
ASSI { 942}
(( segid "PROT" and resid 107 and name HD% ))
(( segid "PROT" and resid 107 and name HA ))
2.700 1.800 1.800 peak 942 weight 0.10000E+01 volume 0.28373E+01 ppm1 7.242 ppm2 3.855
ASSI { 952}
(( segid "PROT" and resid 108 and name HB1 ))
(( segid "PROT" and resid 105 and name HA ))
2.500 1.600 1.600 peak 952 weight 0.10000E+01 volume 0.41582E+01 ppm1 4.018 ppm2 4.352
ASSI { 962}
(( segid "PROT" and resid 108 and name HB1 ))
(( segid "PROT" and resid 108 and name HA ))
2.000 1.000 1.000 peak 962 weight 0.10000E+01 volume 0.16845E+02 ppm1 4.017 ppm2 4.236
ASSI { 972}
(( segid "PROT" and resid 96 and name HB1 ))
(( segid "PROT" and resid 96 and name HA ))
2.700 1.800 1.800 peak 972 weight 0.10000E+01 volume 0.28585E+01 ppm1 3.420 ppm2 3.825
ASSI { 982}
(( segid "PROT" and resid 107 and name HB1 ))
(( segid "PROT" and resid 107 and name HA ))
2.200 1.200 1.200 peak 982 weight 0.10000E+01 volume 0.83628E+01 ppm1 3.093 ppm2 3.855
ASSI { 992}
(( segid "PROT" and resid 96 and name HB2 ))
(( segid "PROT" and resid 96 and name HA ))
2.600 1.700 1.700 peak 992 weight 0.10000E+01 volume 0.34567E+01 ppm1 2.583 ppm2 3.825
ASSI { 1002}
(( segid "PROT" and resid 111 and name HB1 ))
(( segid "PROT" and resid 108 and name HA ))
2.800 2.000 2.000 peak 1002 weight 0.10000E+01 volume 0.21206E+01 ppm1 1.909 ppm2 4.234
ASSI { 1012}
(( segid "PROT" and resid 110 and name HB ))
(( segid "PROT" and resid 107 and name HA ))
2.700 1.800 1.800 peak 1012 weight 0.10000E+01 volume 0.26266E+01 ppm1 1.801 ppm2 3.854
ASSI { 1022}
(( segid "PROT" and resid 111 and name HB2 ))
(( segid "PROT" and resid 108 and name HA ))
2.900 2.100 2.100 peak 1022 weight 0.10000E+01 volume 0.18539E+01 ppm1 1.786 ppm2 4.236
ASSI { 1042}
(( segid "PROT" and resid 110 and name HG11))
(( segid "PROT" and resid 107 and name HA ))
2.400 1.400 1.400 peak 1042 weight 0.10000E+01 volume 0.50798E+01 ppm1 1.154 ppm2 3.857
ASSI { 1052}
(( segid "PROT" and resid 110 and name HG2% ))
(( segid "PROT" and resid 107 and name HA ))
2.800 2.000 2.000 peak 1052 weight 0.10000E+01 volume 0.22040E+01 ppm1 0.695 ppm2 3.855
ASSI { 1062}
(( segid "PROT" and resid 110 and name HD1% ))
(( segid "PROT" and resid 107 and name HA ))
2.600 1.700 1.700 peak 1062 weight 0.10000E+01 volume 0.35344E+01 ppm1 0.569 ppm2 3.856
ASSI { 1072}
(( segid "PROT" and resid 105 and name HD% ))
(( segid "PROT" and resid 105 and name HA ))
2.600 1.700 1.700 peak 1072 weight 0.10000E+01 volume 0.30484E+01 ppm1 7.234 ppm2 4.364
ASSI { 1092}
(( segid "PROT" and resid 88 and name HD% ))
(( segid "PROT" and resid 88 and name HA ))
2.800 2.000 2.000 peak 1092 weight 0.10000E+01 volume 0.19898E+01 ppm1 6.977 ppm2 4.331
ASSI { 1102}
(( segid "PROT" and resid 105 and name HB1 ))
(( segid "PROT" and resid 105 and name HA ))
2.500 1.600 1.600 peak 1102 weight 0.10000E+01 volume 0.44197E+01 ppm1 3.172 ppm2 4.362
ASSI { 1112}
(( segid "PROT" and resid 105 and name HB2 ))
(( segid "PROT" and resid 105 and name HA ))
2.600 1.700 1.700 peak 1112 weight 0.10000E+01 volume 0.34973E+01 ppm1 3.103 ppm2 4.362
ASSI { 1132}
(( segid "PROT" and resid 95 and name HD% ))
(( segid "PROT" and resid 95 and name HA ))
2.900 2.100 2.100 peak 1132 weight 0.10000E+01 volume 0.16794E+01 ppm1 6.869 ppm2 3.647
ASSI { 1142}
(( segid "PROT" and resid 20 and name HB1 ))
(( segid "PROT" and resid 20 and name HA ))
1.900 0.900 0.900 peak 1142 weight 0.10000E+01 volume 0.20468E+02 ppm1 4.099 ppm2 4.330
ASSI { 1152}
(( segid "PROT" and resid 98 and name HB2 ))
(( segid "PROT" and resid 95 and name HA ))
2.900 2.100 2.100 peak 1152 weight 0.10000E+01 volume 0.15905E+01 ppm1 3.054 ppm2 3.651
ASSI { 1162}
(( segid "PROT" and resid 95 and name HB1 ))
(( segid "PROT" and resid 95 and name HA ))
2.800 2.000 2.000 peak 1162 weight 0.10000E+01 volume 0.21842E+01 ppm1 2.947 ppm2 3.649
ASSI { 1192}
(( segid "PROT" and resid 74 and name HD% ))
(( segid "PROT" and resid 74 and name HA ))
2.900 2.100 2.100 peak 1192 weight 0.10000E+01 volume 0.17594E+01 ppm1 6.440 ppm2 3.805
ASSI { 1202}
(( segid "PROT" and resid 74 and name HB1 ))
(( segid "PROT" and resid 74 and name HA ))

```

2.700	1.800	1.800	peak	1202	weight	0.10000E+01	volume	0.25521E+01	ppm1	3.000	ppm2	3.810
ASSI { 1212}												
((segid "PROT" and resid 62 and name HD1))												
((segid "PROT" and resid 59 and name HA))												
2.800	2.000	2.000	peak	1212	weight	0.10000E+01	volume	0.20013E+01	ppm1	2.581	ppm2	4.327
ASSI { 1222}												
((segid "PROT" and resid 74 and name HB2))												
((segid "PROT" and resid 74 and name HA))												
2.700	1.800	1.800	peak	1222	weight	0.10000E+01	volume	0.25019E+01	ppm1	2.428	ppm2	3.801
ASSI { 1232}												
((segid "PROT" and resid 47 and name HD%))												
((segid "PROT" and resid 47 and name HA))												
2.800	2.000	2.000	peak	1232	weight	0.10000E+01	volume	0.19922E+01	ppm1	7.410	ppm2	4.152
ASSI { 1242}												
((segid "PROT" and resid 106 and name HD%))												
((segid "PROT" and resid 106 and name HA))												
2.700	1.800	1.800	peak	1242	weight	0.10000E+01	volume	0.28829E+01	ppm1	6.951	ppm2	4.002
ASSI { 1252}												
((segid "PROT" and resid 32 and name HB1))												
((segid "PROT" and resid 32 and name HA))												
2.500	1.600	1.600	peak	1252	weight	0.10000E+01	volume	0.43254E+01	ppm1	3.639	ppm2	4.422
ASSI { 1262}												
((segid "PROT" and resid 32 and name HB2))												
((segid "PROT" and resid 32 and name HA))												
2.500	1.600	1.600	peak	1262	weight	0.10000E+01	volume	0.45345E+01	ppm1	3.408	ppm2	4.424
ASSI { 1272}												
((segid "PROT" and resid 106 and name HB1))												
((segid "PROT" and resid 106 and name HA))												
2.600	1.700	1.700	peak	1272	weight	0.10000E+01	volume	0.30595E+01	ppm1	3.360	ppm2	3.998
ASSI { 1282}												
((segid "PROT" and resid 47 and name HB1))												
((segid "PROT" and resid 47 and name HA))												
2.600	1.700	1.700	peak	1282	weight	0.10000E+01	volume	0.34928E+01	ppm1	3.244	ppm2	4.144
ASSI { 1292}												
((segid "PROT" and resid 106 and name HB2))												
((segid "PROT" and resid 106 and name HA))												
2.400	1.400	1.400	peak	1292	weight	0.10000E+01	volume	0.47428E+01	ppm1	3.136	ppm2	4.000
ASSI { 1302}												
((segid "PROT" and resid 35 and name HG1))												
((segid "PROT" and resid 32 and name HA))												
2.500	1.600	1.600	peak	1302	weight	0.10000E+01	volume	0.37666E+01	ppm1	2.896	ppm2	4.423
ASSI { 1312}												
((segid "PROT" and resid 47 and name HB2))												
((segid "PROT" and resid 47 and name HA))												
2.700	1.800	1.800	peak	1312	weight	0.10000E+01	volume	0.27409E+01	ppm1	2.846	ppm2	4.145
ASSI { 1322}												
((segid "PROT" and resid 59 and name HG1))												
((segid "PROT" and resid 59 and name HA))												
2.800	2.000	2.000	peak	1322	weight	0.10000E+01	volume	0.20732E+01	ppm1	2.663	ppm2	4.338
ASSI { 1342}												
((segid "PROT" and resid 59 and name HB2))												
((segid "PROT" and resid 59 and name HA))												
2.900	2.100	2.100	peak	1342	weight	0.10000E+01	volume	0.16833E+01	ppm1	1.928	ppm2	4.332
ASSI { 1362}												
((segid "PROT" and resid 58 and name HG2%))												
((segid "PROT" and resid 59 and name HA))												
2.900	2.100	2.100	peak	1362	weight	0.10000E+01	volume	0.17814E+01	ppm1	1.110	ppm2	4.338
ASSI { 1402}												
((segid "PROT" and resid 57 and name HE2))												
((segid "PROT" and resid 57 and name HA))												
2.500	1.600	1.600	peak	1402	weight	0.10000E+01	volume	0.37335E+01	ppm1	2.082	ppm2	3.909
ASSI { 1422}												
((segid "PROT" and resid 115 and name HB2))												
((segid "PROT" and resid 116 and name HA))												
2.500	2.500	2.000	peak	1422	weight	0.10000E+01	volume	0.40056E+01	ppm1	1.620	ppm2	4.238
ASSI { 1452}												
((segid "PROT" and resid 57 and name HB2))												
((segid "PROT" and resid 57 and name HA))												
2.800	2.000	2.000	peak	1452	weight	0.10000E+01	volume	0.21470E+01	ppm1	1.117	ppm2	3.907
ASSI { 1462}												
((segid "PROT" and resid 57 and name HD2))												
((segid "PROT" and resid 57 and name HA))												
2.600	1.700	1.700	peak	1462	weight	0.10000E+01	volume	0.31356E+01	ppm1	0.915	ppm2	3.902
ASSI { 1472}												
((segid "PROT" and resid 67 and name HD%))												
((segid "PROT" and resid 67 and name HA))												
2.800	2.000	2.000	peak	1472	weight	0.10000E+01	volume	0.21386E+01	ppm1	6.321	ppm2	4.108
ASSI { 1482}												
((segid "PROT" and resid 67 and name HB1))												
((segid "PROT" and resid 67 and name HA))												
2.300	1.300	1.300	peak	1482	weight	0.10000E+01	volume	0.60720E+01	ppm1	3.005	ppm2	4.099
ASSI { 1492}												
((segid "PROT" and resid 116 and name HB))												
((segid "PROT" and resid 116 and name HA))												
2.100	1.100	1.100	peak	1492	weight	0.10000E+01	volume	0.10649E+02	ppm1	1.851	ppm2	4.267
ASSI { 1512}												
((segid "PROT" and resid 19 and name HG1))												
((segid "PROT" and resid 19 and name HA))												
2.400	1.400	1.400	peak	1512	weight	0.10000E+01	volume	0.53544E+01	ppm1	1.309	ppm2	3.719

```

ASSI { 1522}
  ( segid "PROT" and resid 63 and name HD2%)
  (( segid "PROT" and resid 19 and name HA ))
  2.700 1.800 1.800 peak 1522 weight 0.10000E+01 volume 0.24664E+01 ppm1 1.088 ppm2 3.720
ASSI { 1542}
  ( segid "PROT" and resid 63 and name HD1%)
  (( segid "PROT" and resid 19 and name HA ))
  2.200 1.200 1.200 peak 1542 weight 0.10000E+01 volume 0.78864E+01 ppm1 0.917 ppm2 3.720
ASSI { 1552}
  ( segid "PROT" and resid 116 and name HG2%)
  (( segid "PROT" and resid 116 and name HA ))
  2.200 1.200 1.200 peak 1552 weight 0.10000E+01 volume 0.85343E+01 ppm1 0.860 ppm2 4.275
ASSI { 1582}
  (( segid "PROT" and resid 107 and name HB1 ))
  (( segid "PROT" and resid 104 and name HA ))
  2.400 1.400 1.400 peak 1582 weight 0.10000E+01 volume 0.52143E+01 ppm1 3.089 ppm2 4.111
ASSI { 1602}
  (( segid "PROT" and resid 103 and name HG1 ))
  (( segid "PROT" and resid 103 and name HA ))
  2.700 1.800 1.800 peak 1602 weight 0.10000E+01 volume 0.23739E+01 ppm1 2.039 ppm2 3.221
ASSI { 1612}
  (( segid "PROT" and resid 104 and name HB1 ))
  (( segid "PROT" and resid 104 and name HA ))
  1.900 0.900 0.900 peak 1612 weight 0.10000E+01 volume 0.22561E+02 ppm1 1.962 ppm2 4.102
ASSI { 1632}
  (( segid "PROT" and resid 103 and name HB1 ))
  (( segid "PROT" and resid 103 and name HA ))
  2.700 1.800 1.800 peak 1632 weight 0.10000E+01 volume 0.24604E+01 ppm1 1.783 ppm2 3.225
ASSI { 1682}
  (( segid "PROT" and resid 103 and name HB2 ))
  (( segid "PROT" and resid 103 and name HA ))
  2.600 1.700 1.700 peak 1682 weight 0.10000E+01 volume 0.35179E+01 ppm1 1.332 ppm2 3.221
ASSI { 1702}
  (( segid "PROT" and resid 116 and name HG12))
  (( segid "PROT" and resid 111 and name HA ))
  2.800 2.000 2.000 peak 1702 weight 0.10000E+01 volume 0.20569E+01 ppm1 0.976 ppm2 4.097
ASSI { 1742}
  (( segid "PROT" and resid 61 and name HG2 ))
  (( segid "PROT" and resid 61 and name HA ))
  2.000 1.000 1.000 peak 1742 weight 0.10000E+01 volume 0.14343E+02 ppm1 2.268 ppm2 4.079
ASSI { 1752}
  (( segid "PROT" and resid 111 and name HB1 ))
  (( segid "PROT" and resid 111 and name HA ))
  1.900 1.900 2.600 peak 1752 weight 0.10000E+01 volume 0.22665E+02 ppm1 1.915 ppm2 4.078
ASSI { 1792}
  (( segid "PROT" and resid 29 and name HG2 ))
  (( segid "PROT" and resid 29 and name HA ))
  2.200 1.200 1.200 peak 1792 weight 0.10000E+01 volume 0.81264E+01 ppm1 2.431 ppm2 4.224
ASSI { 1812}
  (( segid "PROT" and resid 29 and name HB1 ))
  (( segid "PROT" and resid 29 and name HA ))
  1.900 0.900 0.900 peak 1812 weight 0.10000E+01 volume 0.21970E+02 ppm1 2.139 ppm2 4.238
ASSI { 1922}
  ( segid "PROT" and resid 82 and name HD%)
  (( segid "PROT" and resid 82 and name HA ))
  2.500 1.600 1.600 peak 1922 weight 0.10000E+01 volume 0.42297E+01 ppm1 6.693 ppm2 4.214
ASSI { 1932}
  (( segid "PROT" and resid 82 and name HB1 ))
  (( segid "PROT" and resid 82 and name HA ))
  2.500 1.600 1.600 peak 1932 weight 0.10000E+01 volume 0.37394E+01 ppm1 3.128 ppm2 4.216
ASSI { 1952}
  (( segid "PROT" and resid 86 and name HG1 ))
  (( segid "PROT" and resid 86 and name HA ))
  2.700 1.800 1.800 peak 1952 weight 0.10000E+01 volume 0.28775E+01 ppm1 1.344 ppm2 4.264
ASSI { 1962}
  (( segid "PROT" and resid 86 and name HG2 ))
  (( segid "PROT" and resid 86 and name HA ))
  2.700 1.800 1.800 peak 1962 weight 0.10000E+01 volume 0.29223E+01 ppm1 0.165 ppm2 4.263
ASSI { 2022}
  (( segid "PROT" and resid 28 and name HB2 ))
  (( segid "PROT" and resid 28 and name HA ))
  2.600 1.700 1.700 peak 2022 weight 0.10000E+01 volume 0.30612E+01 ppm1 2.817 ppm2 4.021
ASSI { 2032}
  (( segid "PROT" and resid 13 and name HB1 ))
  (( segid "PROT" and resid 13 and name HA ))
  2.000 1.000 1.000 peak 2032 weight 0.10000E+01 volume 0.14730E+02 ppm1 2.191 ppm2 4.217
ASSI { 2042}
  (( segid "PROT" and resid 86 and name HB1 ))
  (( segid "PROT" and resid 86 and name HA ))
  2.500 1.600 1.600 peak 2042 weight 0.10000E+01 volume 0.45267E+01 ppm1 1.810 ppm2 4.265
ASSI { 2052}
  (( segid "PROT" and resid 14 and name HG ))
  (( segid "PROT" and resid 14 and name HA ))
  2.800 2.000 2.000 peak 2052 weight 0.10000E+01 volume 0.19350E+01 ppm1 1.426 ppm2 4.090
ASSI { 2112}
  (( segid "PROT" and resid 87 and name HG2 ))
  (( segid "PROT" and resid 87 and name HA ))
  2.200 1.200 1.200 peak 2112 weight 0.10000E+01 volume 0.95163E+01 ppm1 2.235 ppm2 4.334
ASSI { 2132}

```

```

(( segid "PROT" and resid 80 and name HB1 ))
(( segid "PROT" and resid 80 and name HA ))
2.400 1.400 1.400 peak 2132 weight 0.10000E+01 volume 0.55458E+01 ppm1 2.013 ppm2 4.098
ASSI { 2142}
(( segid "PROT" and resid 68 and name HD% ))
(( segid "PROT" and resid 68 and name HA ))
2.900 2.100 2.100 peak 2142 weight 0.10000E+01 volume 0.18798E+01 ppm1 7 208 ppm2 4.583
ASSI { 2152}
(( segid "PROT" and resid 21 and name HB ))
(( segid "PROT" and resid 18 and name HA ))
2.700 1.800 1.800 peak 2152 weight 0.10000E+01 volume 0.26066E+01 ppm1 1.954 ppm2 3.312
ASSI { 2162}
(( segid "PROT" and resid 73 and name HB2 ))
(( segid "PROT" and resid 73 and name HA ))
2.400 1.400 1.400 peak 2162 weight 0.10000E+01 volume 0.47318E+01 ppm1 1.919 ppm2 4.261
ASSI { 2172}
(( segid "PROT" and resid 18 and name HG ))
(( segid "PROT" and resid 18 and name HA ))
3.000 2.200 2.200 peak 2172 weight 0.10000E+01 volume 0.15478E+01 ppm1 1.708 ppm2 3.315
ASSI { 2182}
(( segid "PROT" and resid 81 and name HB ))
(( segid "PROT" and resid 78 and name HA ))
2.900 2.100 2.100 peak 2182 weight 0.10000E+01 volume 0.16328E+01 ppm1 1.471 ppm2 3.416
ASSI { 2192}
(( segid "PROT" and resid 59 and name HE% ))
(( segid "PROT" and resid 78 and name HA ))
2.800 2.000 2.000 peak 2192 weight 0.10000E+01 volume 0.19929E+01 ppm1 1.311 ppm2 3.422
ASSI { 2212}
(( segid "PROT" and resid 78 and name HB1 ))
(( segid "PROT" and resid 78 and name HA ))
2.600 1.700 1.700 peak 2212 weight 0.10000E+01 volume 0.36430E+01 ppm1 0.739 ppm2 3.417
ASSI { 2242}
(( segid "PROT" and resid 18 and name HD1% ))
(( segid "PROT" and resid 18 and name HA ))
2.700 1.800 1.800 peak 2242 weight 0.10000E+01 volume 0.24789E+01 ppm1 0.511 ppm2 3.318
ASSI { 2282}
(( segid "PROT" and resid 77 and name HB1 ))
(( segid "PROT" and resid 77 and name HA ))
2.500 1.600 1.600 peak 2282 weight 0.10000E+01 volume 0.45855E+01 ppm1 2.749 ppm2 4.395
ASSI { 2292}
(( segid "PROT" and resid 80 and name HB2 ))
(( segid "PROT" and resid 77 and name HA ))
2.700 1.800 1.800 peak 2292 weight 0.10000E+01 volume 0.25994E+01 ppm1 1.942 ppm2 4.393
ASSI { 2302}
(( segid "PROT" and resid 50 and name HG11 ))
(( segid "PROT" and resid 50 and name HA ))
2.900 2.100 2.100 peak 2302 weight 0.10000E+01 volume 0.16293E+01 ppm1 0.837 ppm2 3.951
ASSI { 2312}
(( segid "PROT" and resid 50 and name HD1% ))
(( segid "PROT" and resid 50 and name HA ))
2.100 1.100 1.100 peak 2312 weight 0.10000E+01 volume 0.10702E+02 ppm1 0.582 ppm2 3.952
ASSI { 2342}
(( segid "PROT" and resid 92 and name HG2 ))
(( segid "PROT" and resid 92 and name HA ))
2.300 1.300 1.300 peak 2342 weight 0.10000E+01 volume 0.72564E+01 ppm1 2.257 ppm2 4.253
ASSI { 2352}
(( segid "PROT" and resid 92 and name HB1 ))
(( segid "PROT" and resid 92 and name HA ))
2.200 1.200 1.200 peak 2352 weight 0.10000E+01 volume 0.82085E+01 ppm1 2 103 ppm2 4.253
ASSI { 2362}
(( segid "PROT" and resid 92 and name HB2 ))
(( segid "PROT" and resid 92 and name HA ))
2.300 1.300 1.300 peak 2362 weight 0.10000E+01 volume 0.76333E+01 ppm1 2.023 ppm2 4.252
ASSI { 2372}
(( segid "PROT" and resid 51 and name HB2 ))
(( segid "PROT" and resid 51 and name HA ))
2.200 1.200 1.200 peak 2372 weight 0.10000E+01 volume 0.93999E+01 ppm1 1.212 ppm2 3.878
ASSI { 2402}
(( segid "PROT" and resid 109 and name HB2 ))
(( segid "PROT" and resid 109 and name HA ))
2.500 1.600 1.600 peak 2402 weight 0.10000E+01 volume 0.37867E+01 ppm1 1.586 ppm2 4.072
ASSI { 2412}
(( segid "PROT" and resid 109 and name HD1 ))
(( segid "PROT" and resid 109 and name HA ))
2.200 1.200 1.200 peak 2412 weight 0.10000E+01 volume 0.98857E+01 ppm1 1.421 ppm2 4.069
ASSI { 2422}
(( segid "PROT" and resid 109 and name HG1 ))
(( segid "PROT" and resid 109 and name HA ))
2.700 1.800 1.800 peak 2422 weight 0.10000E+01 volume 0.29134E+01 ppm1 0.852 ppm2 4.074
ASSI { 2432}
(( segid "PROT" and resid 105 and name HB1 ))
(( segid "PROT" and resid 102 and name HA ))
2.600 1.700 1.700 peak 2432 weight 0.10000E+01 volume 0.31410E+01 ppm1 3.172 ppm2 3.721
ASSI { 2442}
(( segid "PROT" and resid 105 and name HB2 ))
(( segid "PROT" and resid 102 and name HA ))
2.600 1.700 1.700 peak 2442 weight 0.10000E+01 volume 0.34157E+01 ppm1 3.110 ppm2 3.725
ASSI { 2452}
(( segid "PROT" and resid 66 and name HD1 ))

```

```

(( segid "PROT" and resid 66 and name HA ))
2.600 1.700 1.700 peak 2452 weight 0.10000E+01 volume 0.34111E+01 ppm1 3.102 ppm2 4.444
ASSI { 2462}
(( segid "PROT" and resid 66 and name HB1 ))
(( segid "PROT" and resid 66 and name HA ))
2.500 1.600 1.600 peak 2462 weight 0.10000E+01 volume 0.45998E+01 ppm1 2.125 ppm2 4.442
ASSI { 2472}
(( segid "PROT" and resid 102 and name HG ))
(( segid "PROT" and resid 102 and name HA ))
2.900 2.100 2.100 peak 2472 weight 0.10000E+01 volume 0.15660E+01 ppm1 1.598 ppm2 3.722
ASSI { 2492}
(( segid "PROT" and resid 102 and name HB2 ))
(( segid "PROT" and resid 102 and name HA ))
2.600 1.700 1.700 peak 2492 weight 0.10000E+01 volume 0.29926E+01 ppm1 1.266 ppm2 3.725
ASSI { 2502}
(( segid "PROT" and resid 101 and name HG2% ))
(( segid "PROT" and resid 102 and name HA ))
2.900 2.100 2.100 peak 2502 weight 0.10000E+01 volume 0.16802E+01 ppm1 1.035 ppm2 3.725
ASSI { 2512}
(( segid "PROT" and resid 102 and name HD2% ))
(( segid "PROT" and resid 102 and name HA ))
2.200 1.200 1.200 peak 2512 weight 0.10000E+01 volume 0.92912E+01 ppm1 0.765 ppm2 3.722
ASSI { 2522}
(( segid "PROT" and resid 42 and name HB1 ))
(( segid "PROT" and resid 42 and name HA ))
2.500 1.600 1.600 peak 2522 weight 0.10000E+01 volume 0.43700E+01 ppm1 2.218 ppm2 4.498
ASSI { 2582}
(( segid "PROT" and resid 6 and name HB1 ))
(( segid "PROT" and resid 6 and name HA ))
2.300 1.300 1.300 peak 2582 weight 0.10000E+01 volume 0.76268E+01 ppm1 1.885 ppm2 4.371
ASSI { 2592}
(( segid "PROT" and resid 6 and name HB2 ))
(( segid "PROT" and resid 6 and name HA ))
2.300 1.300 1.300 peak 2592 weight 0.10000E+01 volume 0.76524E+01 ppm1 1.790 ppm2 4.373
ASSI { 2622}
(( segid "PROT" and resid 34 and name HD% ))
(( segid "PROT" and resid 34 and name HA ))
2.700 1.800 1.800 peak 2622 weight 0.10000E+01 volume 0.27444E+01 ppm1 7.182 ppm2 5.002
ASSI { 2632}
(( segid "PROT" and resid 34 and name HB1 ))
(( segid "PROT" and resid 34 and name HA ))
2.700 1.800 1.800 peak 2632 weight 0.10000E+01 volume 0.28879E+01 ppm1 3.515 ppm2 5.002
ASSI { 2642}
(( segid "PROT" and resid 15 and name HB1 ))
(( segid "PROT" and resid 12 and name HA ))
2.600 1.700 1.700 peak 2642 weight 0.10000E+01 volume 0.32274E+01 ppm1 3.248 ppm2 4.707
ASSI { 2662}
(( segid "PROT" and resid 15 and name HB2 ))
(( segid "PROT" and resid 12 and name HA ))
2.900 2.100 2.100 peak 2662 weight 0.10000E+01 volume 0.16345E+01 ppm1 3.089 ppm2 4.717
ASSI { 2702}
(( segid "PROT" and resid 103 and name HB2 ))
(( segid "PROT" and resid 100 and name HA ))
2.900 2.100 2.100 peak 2702 weight 0.10000E+01 volume 0.16134E+01 ppm1 1.345 ppm2 4.362
ASSI { 2712}
(( segid "PROT" and resid 34 and name HZ ))
(( segid "PROT" and resid 99 and name HA ))
2.800 2.000 2.000 peak 2712 weight 0.10000E+01 volume 0.22850E+01 ppm1 7.294 ppm2 3.915
ASSI { 2742}
(( segid "PROT" and resid 115 and name HB2 ))
(( segid "PROT" and resid 115 and name HA ))
2.200 1.200 1.200 peak 2742 weight 0.10000E+01 volume 0.98559E+01 ppm1 1.608 ppm2 4.256
ASSI { 2772}
(( segid "PROT" and resid 82 and name HD% ))
(( segid "PROT" and resid 99 and name HA ))
2.900 2.100 2.100 peak 2772 weight 0.10000E+01 volume 0.16551E+01 ppm1 6.698 ppm2 3.908
ASSI { 2782}
(( segid "PROT" and resid 84 and name HB1 ))
(( segid "PROT" and resid 84 and name HA ))
2.600 1.700 1.700 peak 2782 weight 0.10000E+01 volume 0.32197E+01 ppm1 3.027 ppm2 4.340
ASSI { 2792}
(( segid "PROT" and resid 84 and name HB2 ))
(( segid "PROT" and resid 84 and name HA ))
2.700 1.800 1.800 peak 2792 weight 0.10000E+01 volume 0.29245E+01 ppm1 2.710 ppm2 4.343
ASSI { 2802}
(( segid "PROT" and resid 87 and name HB1 ))
(( segid "PROT" and resid 84 and name HA ))
2.800 2.000 2.000 peak 2802 weight 0.10000E+01 volume 0.21085E+01 ppm1 2.231 ppm2 4.341
ASSI { 2832}
(( segid "PROT" and resid 79 and name HB2 ))
(( segid "PROT" and resid 76 and name HA ))
2.800 2.000 2.000 peak 2832 weight 0.10000E+01 volume 0.23028E+01 ppm1 2.109 ppm2 4.118
ASSI { 2862}
(( segid "PROT" and resid 52 and name HD% ))
(( segid "PROT" and resid 52 and name HA ))
2.800 2.000 2.000 peak 2862 weight 0.10000E+01 volume 0.23174E+01 ppm1 7.277 ppm2 5.037
ASSI { 2892}
(( segid "PROT" and resid 53 and name HD1 ))
(( segid "PROT" and resid 52 and name HA ))

```

2.400	1.400	1.400	peak	2892	weight	0.10000E+01	volume	0.55449E+01	ppm1	3.654	ppm2	5.038
ASSI { 2902}												
((segid "PROT" and resid 53 and name HD2))												
((segid "PROT" and resid 52 and name HA))												
2.400	1.400	1.400	peak	2902	weight	0.10000E+01	volume	0.48228E+01	ppm1	3.442	ppm2	5.036
ASSI { 2912}												
((segid "PROT" and resid 52 and name HB1))												
((segid "PROT" and resid 52 and name HA))												
2.600	1.700	1.700	peak	2912	weight	0.10000E+01	volume	0.33008E+01	ppm1	3.088	ppm2	5.040
ASSI { 2922}												
((segid "PROT" and resid 52 and name HB2))												
((segid "PROT" and resid 52 and name HA))												
2.700	1.800	1.800	peak	2922	weight	0.10000E+01	volume	0.25314E+01	ppm1	2.964	ppm2	5.037
ASSI { 2952}												
((segid "PROT" and resid 34 and name HD%))												
((segid "PROT" and resid 31 and name HA))												
2.600	1.700	1.700	peak	2952	weight	0.10000E+01	volume	0.33249E+01	ppm1	7.187	ppm2	4.441
ASSI { 2962}												
((segid "PROT" and resid 55 and name HB1))												
((segid "PROT" and resid 55 and name HA))												
2.400	1.400	1.400	peak	2962	weight	0.10000E+01	volume	0.52960E+01	ppm1	2.405	ppm2	4.780
ASSI { 2992}												
((segid "PROT" and resid 102 and name HD1%))												
((segid "PROT" and resid 31 and name HA))												
2.300	1.300	1.300	peak	2992	weight	0.10000E+01	volume	0.69041E+01	ppm1	0.763	ppm2	4.440
ASSI { 3012}												
((segid "PROT" and resid 11 and name HD1))												
((segid "PROT" and resid 10 and name HA))												
2.100	1.100	1.100	peak	3012	weight	0.10000E+01	volume	0.11211E+02	ppm1	3.909	ppm2	4.917
ASSI { 3052}												
((segid "PROT" and resid 90 and name HD1))												
((segid "PROT" and resid 89 and name HA))												
2.500	1.600	1.600	peak	3052	weight	0.10000E+01	volume	0.37580E+01	ppm1	4.115	ppm2	5.088
ASSI { 3062}												
((segid "PROT" and resid 90 and name HD2))												
((segid "PROT" and resid 89 and name HA))												
2.600	1.700	1.700	peak	3062	weight	0.10000E+01	volume	0.34612E+01	ppm1	3.940	ppm2	5.091
ASSI { 3072}												
((segid "PROT" and resid 89 and name HB1))												
((segid "PROT" and resid 89 and name HA))												
2.800	2.000	2.000	peak	3072	weight	0.10000E+01	volume	0.19657E+01	ppm1	3.111	ppm2	5.078
ASSI { 3082}												
((segid "PROT" and resid 89 and name HB2))												
((segid "PROT" and resid 89 and name HA))												
2.900	2.100	2.100	peak	3082	weight	0.10000E+01	volume	0.16124E+01	ppm1	2.904	ppm2	5.088
ASSI { 3092}												
((segid "PROT" and resid 11 and name HA))												
((segid "PROT" and resid 11 and name HD1))												
2.800	2.000	2.000	peak	3092	weight	0.10000E+01	volume	0.19160E+01	ppm1	4.370	ppm2	3.904
ASSI { 3102}												
((segid "PROT" and resid 8 and name HG1))												
((segid "PROT" and resid 8 and name HD1))												
2.100	1.100	1.100	peak	3102	weight	0.10000E+01	volume	0.11827E+02	ppm1	2.074	ppm2	3.882
ASSI { 3112}												
((segid "PROT" and resid 36 and name HA))												
((segid "PROT" and resid 37 and name HD1))												
2.700	1.800	1.800	peak	3112	weight	0.10000E+01	volume	0.28261E+01	ppm1	4.872	ppm2	3.704
ASSI { 3122}												
((segid "PROT" and resid 7 and name HA))												
((segid "PROT" and resid 8 and name HD1))												
2.300	1.300	1.300	peak	3122	weight	0.10000E+01	volume	0.76265E+01	ppm1	4.585	ppm2	3.865
ASSI { 3132}												
((segid "PROT" and resid 7 and name HA))												
((segid "PROT" and resid 8 and name HD2))												
2.300	1.300	1.300	peak	3132	weight	0.10000E+01	volume	0.66114E+01	ppm1	4.587	ppm2	3.716
ASSI { 3142}												
((segid "PROT" and resid 8 and name HD2))												
((segid "PROT" and resid 8 and name HD1))												
1.800	0.800	0.800	peak	3142	weight	0.10000E+01	volume	0.26186E+02	ppm1	3.720	ppm2	3.860
ASSI { 3152}												
((segid "PROT" and resid 37 and name HB1))												
((segid "PROT" and resid 37 and name HD1))												
2.700	1.800	1.800	peak	3152	weight	0.10000E+01	volume	0.28240E+01	ppm1	2.371	ppm2	3.695
ASSI { 3162}												
((segid "PROT" and resid 8 and name HB1))												
((segid "PROT" and resid 8 and name HD1))												
2.900	2.100	2.100	peak	3162	weight	0.10000E+01	volume	0.17476E+01	ppm1	2.298	ppm2	3.866
ASSI { 3172}												
((segid "PROT" and resid 53 and name HG1))												
((segid "PROT" and resid 53 and name HD1))												
2.400	1.400	1.400	peak	3172	weight	0.10000E+01	volume	0.53813E+01	ppm1	2.286	ppm2	3.674
ASSI { 3182}												
((segid "PROT" and resid 37 and name HG1))												
((segid "PROT" and resid 37 and name HD1))												
2.300	1.300	1.300	peak	3182	weight	0.10000E+01	volume	0.67841E+01	ppm1	2.181	ppm2	3.700
ASSI { 3192}												
((segid "PROT" and resid 8 and name HG1))												
((segid "PROT" and resid 8 and name HD2))												
2.200	1.200	1.200	peak	3192	weight	0.10000E+01	volume	0.10002E+02	ppm1	2.053	ppm2	3.717

```

ASSI { 3212}
(( segid "PROT" and resid 37 and name HB2 ))
(( segid "PROT" and resid 37 and name HD1 ))
2.500 1.600 1.600 peak 3212 weight 0.10000E+01 volume 0.40424E+01 ppm1 1.710 ppm2 3.686
ASSI { 3262}
(( segid "PROT" and resid 43 and name HA ))
(( segid "PROT" and resid 44 and name HD2 ))
2.400 1.400 1.400 peak 3262 weight 0.10000E+01 volume 0.56600E+01 ppm1 4.992 ppm2 3.570
ASSI { 3282}
(( segid "PROT" and resid 90 and name HD2 ))
(( segid "PROT" and resid 90 and name HD1 ))
2.500 1.600 1.600 peak 3282 weight 0.10000E+01 volume 0.38203E+01 ppm1 3.937 ppm2 4.103
ASSI { 3292}
(( segid "PROT" and resid 44 and name HD1 ))
(( segid "PROT" and resid 44 and name HD2 ))
2.100 1.100 1.100 peak 3292 weight 0.10000E+01 volume 0.11588E+02 ppm1 3.826 ppm2 3.570
ASSI { 3302}
(( segid "PROT" and resid 53 and name HD1 ))
(( segid "PROT" and resid 53 and name HD2 ))
2.100 1.100 1.100 peak 3302 weight 0.10000E+01 volume 0.11080E+02 ppm1 3.654 ppm2 3.447
ASSI { 3332}
(( segid "PROT" and resid 53 and name HG1 ))
(( segid "PROT" and resid 53 and name HD2 ))
2.600 1.700 1.700 peak 3332 weight 0.10000E+01 volume 0.34260E+01 ppm1 2.280 ppm2 3.443
ASSI { 3342}
(( segid "PROT" and resid 44 and name HG1 ))
(( segid "PROT" and resid 44 and name HD1 ))
2.500 1.600 1.600 peak 3342 weight 0.10000E+01 volume 0.38679E+01 ppm1 2.211 ppm2 3.827
ASSI { 3352}
(( segid "PROT" and resid 44 and name HG1 ))
(( segid "PROT" and resid 44 and name HD2 ))
2.500 1.600 1.600 peak 3352 weight 0.10000E+01 volume 0.38481E+01 ppm1 2 209 ppm2 3.573
ASSI { 3362}
(( segid "PROT" and resid 90 and name HB2 ))
(( segid "PROT" and resid 90 and name HD1 ))
2.800 2.000 2.000 peak 3362 weight 0.10000E+01 volume 0.20486E+01 ppm1 2.199 ppm2 4.116
ASSI { 3372}
(( segid "PROT" and resid 90 and name HB2 ))
(( segid "PROT" and resid 90 and name HD2 ))
2.700 1.800 1.800 peak 3372 weight 0.10000E+01 volume 0.25162E+01 ppm1 2.199 ppm2 3.945
ASSI { 3382}
(( segid "PROT" and resid 44 and name HB2 ))
(( segid "PROT" and resid 44 and name HD2 ))
2.500 1.600 1.600 peak 3382 weight 0.10000E+01 volume 0.45799E+01 ppm1 2.077 ppm2 3.574
ASSI { 3392}
(( segid "PROT" and resid 53 and name HG2 ))
(( segid "PROT" and resid 53 and name HD2 ))
2.700 1.800 1.800 peak 3392 weight 0.10000E+01 volume 0.26881E+01 ppm1 1.943 ppm2 3.442
ASSI { 3412}
(( segid "PROT" and resid 33 and name HD1 ))
(( segid "PROT" and resid 33 and name HD2 ))
2.500 1.600 1.600 peak 3412 weight 0.10000E+01 volume 0.46632E+01 ppm1 2.268 ppm2 1.576
ASSI { 3432}
(( segid "PROT" and resid 44 and name HD1 ))
(( segid "PROT" and resid 43 and name HA ))
2.400 1.400 1.400 peak 3432 weight 0.10000E+01 volume 0.53974E+01 ppm1 3.826 ppm2 4.987
ASSI { 3462}
(( segid "PROT" and resid 114 and name HA1 ))
(( segid "PROT" and resid 114 and name HA2 ))
2.100 1.100 1.100 peak 3462 weight 0.10000E+01 volume 0.10591E+02 ppm1 4.258 ppm2 4.070
ASSI { 3492}
(( segid "PROT" and resid 37 and name HA ))
(( segid "PROT" and resid 55 and name HB1 ))
2.900 2.100 2.100 peak 3492 weight 0.10000E+01 volume 0.16441E+01 ppm1 4.278 ppm2 2.404
ASSI { 3512}
(( segid "PROT" and resid 57 and name HE2 ))
(( segid "PROT" and resid 57 and name HE1 ))
2.300 1.300 1.300 peak 3512 weight 0.10000E+01 volume 0.74338E+01 ppm1 2.077 ppm2 2.615
ASSI { 3522}
(( segid "PROT" and resid 57 and name HD1 ))
(( segid "PROT" and resid 57 and name HE1 ))
2.800 2.000 2.000 peak 3522 weight 0.10000E+01 volume 0.20286E+01 ppm1 1.759 ppm2 2.624
ASSI { 3552}
(( segid "PROT" and resid 57 and name HD2 ))
(( segid "PROT" and resid 57 and name HE1 ))
2.900 2.100 2.100 peak 3552 weight 0.10000E+01 volume 0.16708E+01 ppm1 0.917 ppm2 2.626
ASSI { 3572}
(( segid "PROT" and resid 68 and name HD% ))
(( segid "PROT" and resid 73 and name HB2 ))
2.900 2.100 2.100 peak 3572 weight 0.10000E+01 volume 0.16761E+01 ppm1 7.210 ppm2 1.912
ASSI { 3582}
(( segid "PROT" and resid 68 and name HD% ))
(( segid "PROT" and resid 73 and name HB1 ))
2.800 2.000 2.000 peak 3582 weight 0.10000E+01 volume 0.21142E+01 ppm1 7.199 ppm2 2.025
ASSI { 3612}
(( segid "PROT" and resid 73 and name HA ))
(( segid "PROT" and resid 73 and name HB1 ))
2.600 1.700 1.700 peak 3612 weight 0.10000E+01 volume 0.31935E+01 ppm1 4.261 ppm2 2.026
ASSI { 3632}

```



```

(( segid "PROT" and resid 73 and name HB1 ))
(( segid "PROT" and resid 73 and name HB2 ))
2.200 1.200 1.200 peak 3632 weight 0.10000E+01 volume 0.94680E+01 ppm1 2.031 ppm2 1.912
ASSI { 3652}
(( segid "PROT" and resid 73 and name HG ))
(( segid "PROT" and resid 73 and name HB1 ))
2.400 1.400 1.400 peak 3652 weight 0.10000E+01 volume 0.56300E+01 ppm1 1.804 ppm2 2.035
ASSI { 3662}
(( segid "PROT" and resid 73 and name HG ))
(( segid "PROT" and resid 73 and name HB2 ))
2.500 1.600 1.600 peak 3662 weight 0.10000E+01 volume 0.38407E+01 ppm1 1.805 ppm2 1.924
ASSI { 3702}
(( segid "PROT" and resid 9 and name HA ))
(( segid "PROT" and resid 9 and name HD1 ))
2.600 1.700 1.700 peak 3702 weight 0.10000E+01 volume 0.35675E+01 ppm1 4.368 ppm2 3.223
ASSI { 3752}
(( segid "PROT" and resid 80 and name HA ))
(( segid "PROT" and resid 80 and name HD2 ))
2.400 1.400 1.400 peak 3752 weight 0.10000E+01 volume 0.48838E+01 ppm1 4.096 ppm2 3.319
ASSI { 3762}
(( segid "PROT" and resid 80 and name HA ))
(( segid "PROT" and resid 80 and name HD1 ))
2.800 2.000 2.000 peak 3762 weight 0.10000E+01 volume 0.20750E+01 ppm1 4.096 ppm2 3.401
ASSI { 3772}
(( segid "PROT" and resid 80 and name HB1 ))
(( segid "PROT" and resid 80 and name HD1 ))
2.700 1.800 1.800 peak 3772 weight 0.10000E+01 volume 0.25765E+01 ppm1 2.006 ppm2 3.398
ASSI { 3782}
(( segid "PROT" and resid 80 and name HB1 ))
(( segid "PROT" and resid 80 and name HD2 ))
2.700 1.800 1.800 peak 3782 weight 0.10000E+01 volume 0.27643E+01 ppm1 2.008 ppm2 3.325
ASSI { 3792}
(( segid "PROT" and resid 80 and name HG1 ))
(( segid "PROT" and resid 80 and name HD1 ))
2.300 1.300 1.300 peak 3792 weight 0.10000E+01 volume 0.65114E+01 ppm1 1.786 ppm2 3.404
ASSI { 3802}
(( segid "PROT" and resid 80 and name HG1 ))
(( segid "PROT" and resid 80 and name HD2 ))
2.400 1.400 1.400 peak 3802 weight 0.10000E+01 volume 0.57598E+01 ppm1 1.784 ppm2 3.325
ASSI { 3822}
(( segid "PROT" and resid 110 and name HB ))
(( segid "PROT" and resid 115 and name HB2 ))
2.400 1.400 1.400 peak 3822 weight 0.10000E+01 volume 0.52191E+01 ppm1 1.784 ppm2 1.605
ASSI { 3842}
(( segid "PROT" and resid 115 and name HD1% ))
(( segid "PROT" and resid 115 and name HB2 ))
2.100 1.100 1.100 peak 3842 weight 0.10000E+01 volume 0.10686E+02 ppm1 0.759 ppm2 1.614
ASSI { 3902}
(( segid "PROT" and resid 51 and name HA ))
(( segid "PROT" and resid 51 and name HD1 ))
2.500 1.600 1.600 peak 3902 weight 0.10000E+01 volume 0.38455E+01 ppm1 3.878 ppm2 3.021
ASSI { 3912}
(( segid "PROT" and resid 51 and name HG1 ))
(( segid "PROT" and resid 51 and name HD1 ))
2.200 1.200 1.200 peak 3912 weight 0.10000E+01 volume 0.82005E+01 ppm1 1.353 ppm2 3.022
ASSI { 3922}
(( segid "PROT" and resid 51 and name HG2 ))
(( segid "PROT" and resid 51 and name HD1 ))
2.200 1.200 1.200 peak 3922 weight 0.10000E+01 volume 0.97970E+01 ppm1 1.200 ppm2 3.022
ASSI { 3972}
(( segid "PROT" and resid 109 and name HA ))
(( segid "PROT" and resid 109 and name HE2 ))
2.800 2.000 2.000 peak 3972 weight 0.10000E+01 volume 0.19750E+01 ppm1 4.072 ppm2 2.476
ASSI { 3982}
(( segid "PROT" and resid 109 and name HE1 ))
(( segid "PROT" and resid 109 and name HE2 ))
1.900 0.900 0.900 peak 3982 weight 0.10000E+01 volume 0.18921E+02 ppm1 2.617 ppm2 2.486
ASSI { 4002}
(( segid "PROT" and resid 63 and name HB2 ))
(( segid "PROT" and resid 63 and name HB1 ))
2.400 1.400 1.400 peak 4002 weight 0.10000E+01 volume 0.52005E+01 ppm1 1.969 ppm2 2.354
ASSI { 4012}
(( segid "PROT" and resid 63 and name HG ))
(( segid "PROT" and resid 63 and name HB1 ))
2.700 1.800 1.800 peak 4012 weight 0.10000E+01 volume 0.29071E+01 ppm1 1.854 ppm2 2.356
ASSI { 4022}
(( segid "PROT" and resid 63 and name HG ))
(( segid "PROT" and resid 63 and name HB2 ))
2.900 2.100 2.100 peak 4022 weight 0.10000E+01 volume 0.17630E+01 ppm1 1.851 ppm2 1.979
ASSI { 4032}
(( segid "PROT" and resid 109 and name HD1 ))
(( segid "PROT" and resid 109 and name HE1 ))
2.500 1.600 1.600 peak 4032 weight 0.10000E+01 volume 0.45997E+01 ppm1 1.422 ppm2 2.620
ASSI { 4042}
(( segid "PROT" and resid 109 and name HD1 ))
(( segid "PROT" and resid 109 and name HE2 ))
2.400 1.400 1.400 peak 4042 weight 0.10000E+01 volume 0.47654E+01 ppm1 1.422 ppm2 2.475
ASSI { 4092}
(( segid "PROT" and resid 109 and name HG1 ))

```

1.0000E+01 volume 0.27075E+01 ppm1 0.852 ppm2 2.483
 0.10000E+01 volume 0.31579E+01 ppm1 0.846 ppm2 2.624
 0.10000E+01 volume 0.12880E+02 ppm1 1.452 ppm2 3.036
 0.10000E+01 volume 0.16565E+01 ppm1 6.485 ppm2 1.468
 0.10000E+01 volume 0.27856E+01 ppm1 4.153 ppm2 1.731
 0.10000E+01 volume 0.24930E+01 ppm1 3.720 ppm2 1.476
 0.10000E+01 volume 0.66173E+01 ppm1 2.133 ppm2 1.733
 0.10000E+01 volume 0.24653E+01 ppm1 1.593 ppm2 1.264
 0.10000E+01 volume 0.76368E+01 ppm1 1.471 ppm2 1.265
 0.10000E+01 volume 0.60665E+01 ppm1 0.763 ppm2 1.471
 0.10000E+01 volume 0.40905E+01 ppm1 4.918 ppm2 2.800
 0.10000E+01 volume 0.33594E+01 ppm1 4.604 ppm2 2.737
 0.10000E+01 volume 0.17695E+01 ppm1 4.604 ppm2 2.577
 0.10000E+01 volume 0.35230E+01 ppm1 3.901 ppm2 2.734
 0.10000E+01 volume 0.26744E+02 ppm1 2.728 ppm2 2.582
 0.10000E+01 volume 0.44685E+01 ppm1 1.914 ppm2 2.943
 0.10000E+01 volume 0.23547E+01 ppm1 4.338 ppm2 2.108
 0.10000E+01 volume 0.20197E+01 ppm1 4.339 ppm2 1.457
 0.10000E+01 volume 0.36040E+01 ppm1 2.107 ppm2 1.443
 0.10000E+01 volume 0.84236E+01 ppm1 1.892 ppm2 1.594
 0.10000E+01 volume 0.81373E+01 ppm1 0.844 ppm2 1.888
 0.10000E+01 volume 0.84093E+01 ppm1 0.842 ppm2 1.595

```

(( segid "PROT" and resid 109 and name HE2 ))
2.700 1.800 1.800 peak 4092 weight 0.10000E+01 volume 0.27075E+01 ppm1 0.852 ppm2 2.483
ASSI { 4102}
(( segid "PROT" and resid 109 and name HG1 ))
(( segid "PROT" and resid 109 and name HB1 ))
2.600 1.700 1.700 peak 4102 weight 0.10000E+01 volume 0.31579E+01 ppm1 0.846 ppm2 2.624
ASSI { 4202}
(( segid "PROT" and resid 104 and name HG2 ))
(( segid "PROT" and resid 104 and name HB1 ))
2.100 1.100 1.100 peak 4202 weight 0.10000E+01 volume 0.12880E+02 ppm1 1.452 ppm2 3.036
ASSI { 4312}
(( segid "PROT" and resid 82 and name HE% ))
(( segid "PROT" and resid 102 and name HB1 ))
2.900 2.100 2.100 peak 4312 weight 0.10000E+01 volume 0.16565E+01 ppm1 6.485 ppm2 1.468
ASSI { 4322}
(( segid "PROT" and resid 22 and name HA ))
(( segid "PROT" and resid 22 and name HB2 ))
2.700 1.800 1.800 peak 4322 weight 0.10000E+01 volume 0.27856E+01 ppm1 4.153 ppm2 1.731
ASSI { 4342}
(( segid "PROT" and resid 102 and name HA ))
(( segid "PROT" and resid 102 and name HB1 ))
2.700 1.800 1.800 peak 4342 weight 0.10000E+01 volume 0.24930E+01 ppm1 3.720 ppm2 1.476
ASSI { 4352}
(( segid "PROT" and resid 22 and name HB1 ))
(( segid "PROT" and resid 22 and name HB2 ))
2.300 1.300 1.300 peak 4352 weight 0.10000E+01 volume 0.66173E+01 ppm1 2.133 ppm2 1.733
ASSI { 4372}
(( segid "PROT" and resid 102 and name HG ))
(( segid "PROT" and resid 102 and name HB2 ))
2.700 1.800 1.800 peak 4372 weight 0.10000E+01 volume 0.24653E+01 ppm1 1.593 ppm2 1.264
ASSI { 4382}
(( segid "PROT" and resid 102 and name HB1 ))
(( segid "PROT" and resid 102 and name HB2 ))
2.300 1.300 1.300 peak 4382 weight 0.10000E+01 volume 0.76368E+01 ppm1 1.471 ppm2 1.265
ASSI { 4432}
(( segid "PROT" and resid 102 and name HD2% ))
(( segid "PROT" and resid 102 and name HB1 ))
2.300 1.300 1.300 peak 4432 weight 0.10000E+01 volume 0.60665E+01 ppm1 0.763 ppm2 1.471
ASSI { 4452}
(( segid "PROT" and resid 10 and name HA ))
(( segid "PROT" and resid 10 and name HB1 ))
2.500 1.600 1.600 peak 4452 weight 0.10000E+01 volume 0.40905E+01 ppm1 4.918 ppm2 2.800
ASSI { 4462}
(( segid "PROT" and resid 117 and name HA ))
(( segid "PROT" and resid 117 and name HB1 ))
2.600 1.700 1.700 peak 4462 weight 0.10000E+01 volume 0.33594E+01 ppm1 4.604 ppm2 2.737
ASSI { 4472}
(( segid "PROT" and resid 117 and name HA ))
(( segid "PROT" and resid 117 and name HB2 ))
2.900 2.100 2.100 peak 4472 weight 0.10000E+01 volume 0.17695E+01 ppm1 4.604 ppm2 2.577
ASSI { 4482}
(( segid "PROT" and resid 11 and name HD1 ))
(( segid "PROT" and resid 10 and name HB2 ))
2.600 1.700 1.700 peak 4482 weight 0.10000E+01 volume 0.35230E+01 ppm1 3.901 ppm2 2.734
ASSI { 4492}
(( segid "PROT" and resid 117 and name HB1 ))
(( segid "PROT" and resid 117 and name HB2 ))
1.800 0.800 0.800 peak 4492 weight 0.10000E+01 volume 0.26744E+02 ppm1 2.728 ppm2 2.582
ASSI { 4512}
(( segid "PROT" and resid 111 and name HB1 ))
(( segid "PROT" and resid 111 and name HE1 ))
2.500 1.600 1.600 peak 4512 weight 0.10000E+01 volume 0.44685E+01 ppm1 1.914 ppm2 2.943
ASSI { 4532}
(( segid "PROT" and resid 35 and name HA ))
(( segid "PROT" and resid 56 and name HB1 ))
2.800 2.000 2.000 peak 4532 weight 0.10000E+01 volume 0.23547E+01 ppm1 4.338 ppm2 2.108
ASSI { 4542}
(( segid "PROT" and resid 35 and name HA ))
(( segid "PROT" and resid 56 and name HB2 ))
2.800 2.000 2.000 peak 4542 weight 0.10000E+01 volume 0.20197E+01 ppm1 4.339 ppm2 1.457
ASSI { 4592}
(( segid "PROT" and resid 56 and name HB1 ))
(( segid "PROT" and resid 56 and name HB2 ))
2.600 1.700 1.700 peak 4592 weight 0.10000E+01 volume 0.36040E+01 ppm1 2.107 ppm2 1.443
ASSI { 4602}
(( segid "PROT" and resid 14 and name HB1 ))
(( segid "PROT" and resid 14 and name HB2 ))
2.200 1.200 1.200 peak 4602 weight 0.10000E+01 volume 0.84236E+01 ppm1 1.892 ppm2 1.594
ASSI { 4702}
(( segid "PROT" and resid 14 and name HD1% ))
(( segid "PROT" and resid 14 and name HB1 ))
2.200 1.200 1.200 peak 4702 weight 0.10000E+01 volume 0.81373E+01 ppm1 0.844 ppm2 1.888
ASSI { 4712}
(( segid "PROT" and resid 14 and name HD2% ))
(( segid "PROT" and resid 14 and name HB2 ))
2.200 1.200 1.200 peak 4712 weight 0.10000E+01 volume 0.84093E+01 ppm1 0.842 ppm2 1.595
ASSI { 4752}
(( segid "PROT" and resid 88 and name HD% ))
(( segid "PROT" and resid 88 and name HB1 ))

```

2.800	2.000	2.000	peak	4752	weight	0.10000E+01	volume	0.23178E+01	ppm1	6.968	ppm2	2.964
ASSI { 4752}												
((segid "PROT" and resid 12 and name HA))												
((segid "PROT" and resid 12 and name HB1))												
2.400	1.400	1.400	peak	4762	weight	0.10000E+01	volume	0.54235E+01	ppm1	4.724	ppm2	2.848
ASSI { 4772}												
((segid "PROT" and resid 88 and name HA))												
((segid "PROT" and resid 88 and name HB1))												
2.600	1.700	1.700	peak	4772	weight	0.10000E+01	volume	0.29527E+01	ppm1	4.328	ppm2	2.958
ASSI { 4782}												
(segid "PROT" and resid 67 and name HD%)												
((segid "PROT" and resid 67 and name HB1))												
2.800	2.000	2.000	peak	4782	weight	0.10000E+01	volume	0.21224E+01	ppm1	6.328	ppm2	3.002
ASSI { 4792}												
(segid "PROT" and resid 67 and name HD%)												
((segid "PROT" and resid 67 and name HB2))												
2.900	2.100	2.100	peak	4792	weight	0.10000E+01	volume	0.16139E+01	ppm1	6.323	ppm2	2.095
ASSI { 4812}												
((segid "PROT" and resid 67 and name HA))												
((segid "PROT" and resid 67 and name HB2))												
2.700	1.800	1.800	peak	4812	weight	0.10000E+01	volume	0.23919E+01	ppm1	4.100	ppm2	2.095
ASSI { 4832}												
((segid "PROT" and resid 67 and name HB2))												
((segid "PROT" and resid 67 and name HB1))												
2.400	1.400	1.400	peak	4832	weight	0.10000E+01	volume	0.59989E+01	ppm1	2.093	ppm2	3.004
ASSI { 4842}												
(segid "PROT" and resid 96 and name HD%)												
((segid "PROT" and resid 96 and name HB2))												
3.000	2.200	2.200	peak	4842	weight	0.10000E+01	volume	0.13526E+01	ppm1	7.152	ppm2	2.580
ASSI { 4882}												
((segid "PROT" and resid 96 and name HB1))												
((segid "PROT" and resid 96 and name HB2))												
2.400	1.400	1.400	peak	4882	weight	0.10000E+01	volume	0.48230E+01	ppm1	3.422	ppm2	2.580
ASSI { 4922}												
(segid "PROT" and resid 59 and name HE%)												
((segid "PROT" and resid 78 and name HB1))												
2.800	2.000	2.000	peak	4922	weight	0.10000E+01	volume	0.22267E+01	ppm1	1.310	ppm2	0.747
ASSI { 4942}												
((segid "PROT" and resid 78 and name HB1))												
((segid "PROT" and resid 78 and name HB2))												
2.100	1.100	1.100	peak	4942	weight	0.10000E+01	volume	0.11151E+02	ppm1	0.741	ppm2	0.466
ASSI { 5002}												
(segid "PROT" and resid 74 and name HD%)												
((segid "PROT" and resid 74 and name HB1))												
2.800	2.000	2.000	peak	5002	weight	0.10000E+01	volume	0.21667E+01	ppm1	6.439	ppm2	3.002
ASSI { 5012}												
(segid "PROT" and resid 74 and name HD%)												
((segid "PROT" and resid 74 and name HB2))												
2.800	2.000	2.000	peak	5012	weight	0.10000E+01	volume	0.19346E+01	ppm1	6.429	ppm2	2.428
ASSI { 5092}												
((segid "PROT" and resid 74 and name HB1))												
((segid "PROT" and resid 74 and name HB2))												
2.400	1.400	1.400	peak	5092	weight	0.10000E+01	volume	0.52357E+01	ppm1	2.997	ppm2	2.425
ASSI { 5102}												
((segid "PROT" and resid 46 and name HB1))												
((segid "PROT" and resid 46 and name HB2))												
2.500	1.600	1.600	peak	5102	weight	0.10000E+01	volume	0.39310E+01	ppm1	2.759	ppm2	2.426
ASSI { 5132}												
((segid "PROT" and resid 18 and name HB1))												
((segid "PROT" and resid 18 and name HB2))												
2.500	1.600	1.600	peak	5132	weight	0.10000E+01	volume	0.40166E+01	ppm1	1.562	ppm2	0.344
ASSI { 5172}												
((segid "PROT" and resid 116 and name HG12%))												
((segid "PROT" and resid 116 and name HB))												
2.800	2.000	2.000	peak	5172	weight	0.10000E+01	volume	0.21986E+01	ppm1	0.966	ppm2	1.847
ASSI { 5182}												
(segid "PROT" and resid 116 and name HG2%)												
((segid "PROT" and resid 116 and name HB))												
2.100	1.100	1.100	peak	5182	weight	0.10000E+01	volume	0.12445E+02	ppm1	0.861	ppm2	1.847
ASSI { 5192}												
(segid "PROT" and resid 18 and name HD1%)												
((segid "PROT" and resid 74 and name HB1))												
3.000	2.200	2.200	peak	5192	weight	0.10000E+01	volume	0.15029E+01	ppm1	0.513	ppm2	3.005
ASSI { 5262}												
(segid "PROT" and resid 34 and name HD%)												
((segid "PROT" and resid 34 and name HB1))												
2.900	2.100	2.100	peak	5262	weight	0.10000E+01	volume	0.18411E+01	ppm1	7.188	ppm2	3.521
ASSI { 5272}												
(segid "PROT" and resid 34 and name HD%)												
((segid "PROT" and resid 34 and name HB2))												
2.800	2.000	2.000	peak	5272	weight	0.10000E+01	volume	0.19384E+01	ppm1	7.190	ppm2	2.628
ASSI { 5292}												
((segid "PROT" and resid 34 and name HA))												
((segid "PROT" and resid 34 and name HB2))												
2.800	2.000	2.000	peak	5292	weight	0.10000E+01	volume	0.19990E+01	ppm1	4.999	ppm2	2.642
ASSI { 5312}												
((segid "PROT" and resid 34 and name HB1))												
((segid "PROT" and resid 34 and name HB2))												
2.500	1.600	1.600	peak	5312	weight	0.10000E+01	volume	0.39383E+01	ppm1	3.516	ppm2	2.634

```

ASSI { 5332}
( segid "PROT" and resid 56 and name HD1% )
(( segid "PROT" and resid 34 and name HB1 ))
2.900 2.100 2.100 peak 5332 weight 0.10000E+01 volume 0.16847E+01 ppm1 0.978 ppm2 3.522
ASSI { 5352}
( segid "PROT" and resid 102 and name HD2% )
(( segid "PROT" and resid 105 and name HB1 ))
2.800 2.000 2.000 peak 5352 weight 0.10000E+01 volume 0.21496E+01 ppm1 0.768 ppm2 3.140
ASSI { 5372}
(( segid "PROT" and resid 98 and name HA ))
(( segid "PROT" and resid 101 and name HB ))
2.600 1.700 1.700 peak 5372 weight 0.10000E+01 volume 0.34216E+01 ppm1 4.223 ppm2 1.942
ASSI { 5412}
( segid "PROT" and resid 106 and name HD% )
(( segid "PROT" and resid 106 and name HB1 ))
2.800 2.000 2.000 peak 5412 weight 0.10000E+01 volume 0.23568E+01 ppm1 6.952 ppm2 3.355
ASSI { 5422}
( segid "PROT" and resid 106 and name HD% )
(( segid "PROT" and resid 106 and name HB2 ))
2.700 1.800 1.800 peak 5422 weight 0.10000E+01 volume 0.27113E+01 ppm1 6.948 ppm2 3.135
ASSI { 5432}
(( segid "PROT" and resid 100 and name HA ))
(( segid "PROT" and resid 100 and name HB2 ))
2.300 1.300 1.300 peak 5432 weight 0.10000E+01 volume 0.75634E+01 ppm1 4.370 ppm2 2.851
ASSI { 5442}
(( segid "PROT" and resid 100 and name HA ))
(( segid "PROT" and resid 100 and name HB1 ))
2.300 1.300 1.300 peak 5442 weight 0.10000E+01 volume 0.77384E+01 ppm1 4.368 ppm2 2.916
ASSI { 5452}
(( segid "PROT" and resid 97 and name HA ))
(( segid "PROT" and resid 100 and name HB1 ))
2.600 1.700 1.700 peak 5452 weight 0.10000E+01 volume 0.33747E+01 ppm1 4.235 ppm2 2.901
ASSI { 5462}
(( segid "PROT" and resid 97 and name HA ))
(( segid "PROT" and resid 100 and name HB2 ))
2.500 1.600 1.600 peak 5462 weight 0.10000E+01 volume 0.37542E+01 ppm1 4.236 ppm2 2.848
ASSI { 5502}
(( segid "PROT" and resid 80 and name HD1 ))
(( segid "PROT" and resid 52 and name HB2 ))
2.900 2.100 2.100 peak 5502 weight 0.10000E+01 volume 0.18956E+01 ppm1 3.411 ppm2 2.955
ASSI { 5512}
(( segid "PROT" and resid 106 and name HB1 ))
(( segid "PROT" and resid 106 and name HB2 ))
2.300 1.300 1.300 peak 5512 weight 0.10000E+01 volume 0.76377E+01 ppm1 3.354 ppm2 3.134
ASSI { 5522}
(( segid "PROT" and resid 80 and name HD2 ))
(( segid "PROT" and resid 52 and name HB2 ))
3.000 2.200 2.200 peak 5522 weight 0.10000E+01 volume 0.15004E+01 ppm1 3.331 ppm2 2.955
ASSI { 5542}
(( segid "PROT" and resid 95 and name HB2 ))
(( segid "PROT" and resid 95 and name HB1 ))
2.400 1.400 1.400 peak 5542 weight 0.10000E+01 volume 0.54751E+01 ppm1 2.639 ppm2 2.953
ASSI { 5572}
( segid "PROT" and resid 52 and name HD% )
(( segid "PROT" and resid 52 and name HB2 ))
2.700 1.800 1.800 peak 5572 weight 0.10000E+01 volume 0.25372E+01 ppm1 7.280 ppm2 2.968
ASSI { 5582}
( segid "PROT" and resid 52 and name HD% )
(( segid "PROT" and resid 52 and name HB1 ))
2.500 1.600 1.600 peak 5582 weight 0.10000E+01 volume 0.40623E+01 ppm1 7.278 ppm2 3.094
ASSI { 5592}
( segid "PROT" and resid 15 and name HD% )
(( segid "PROT" and resid 15 and name HB2 ))
2.800 2.000 2.000 peak 5592 weight 0.10000E+01 volume 0.22258E+01 ppm1 7.107 ppm2 3.091
ASSI { 5602}
( segid "PROT" and resid 15 and name HD% )
(( segid "PROT" and resid 15 and name HB1 ))
2.800 2.000 2.000 peak 5602 weight 0.10000E+01 volume 0.20171E+01 ppm1 7.104 ppm2 3.242
ASSI { 5662}
(( segid "PROT" and resid 15 and name HB1 ))
(( segid "PROT" and resid 15 and name HB2 ))
2.200 1.200 1.200 peak 5662 weight 0.10000E+01 volume 0.10177E+02 ppm1 3.237 ppm2 3.094
ASSI { 5722}
( segid "PROT" and resid 82 and name HD% )
(( segid "PROT" and resid 82 and name HB1 ))
2.700 1.800 1.800 peak 5722 weight 0.10000E+01 volume 0.25453E+01 ppm1 6.693 ppm2 3.141
ASSI { 5732}
( segid "PROT" and resid 82 and name HD% )
(( segid "PROT" and resid 82 and name HB2 ))
2.800 2.000 2.000 peak 5732 weight 0.10000E+01 volume 0.21571E+01 ppm1 6.691 ppm2 3.009
ASSI { 5772}
(( segid "PROT" and resid 84 and name HB2 ))
(( segid "PROT" and resid 84 and name HB1 ))
2.300 1.300 1.300 peak 5772 weight 0.10000E+01 volume 0.65685E+01 ppm1 2.715 ppm2 3.014
ASSI { 5852}
(( segid "PROT" and resid 92 and name HA ))
(( segid "PROT" and resid 92 and name HG1 ))
2.400 1.400 1.400 peak 5852 weight 0.10000E+01 volume 0.57224E+01 ppm1 4.255 ppm2 2.387
ASSI { 5882}

```

```

(( segid "PROT" and resid 103 and name HA ))
(( segid "PROT" and resid 103 and name HG2 ))
2.700 1.800 1.800 peak 5882 weight 0.10000E+01 volume 0.24953E+01 ppm1 3.225 ppm2 1.964
ASSI { 5922}
(( segid "PROT" and resid 110 and name HG11))
(( segid "PROT" and resid 110 and name HB ))
2.600 1.700 1.700 peak 5922 weight 0.10000E+01 volume 0.29669E+01 ppm1 1.151 ppm2 1.796
ASSI { 5932}
(( segid "PROT" and resid 110 and name HG12))
(( segid "PROT" and resid 110 and name HB ))
2.700 1.800 1.800 peak 5932 weight 0.10000E+01 volume 0.28889E+01 ppm1 1.092 ppm2 1.795
ASSI { 5992}
(( segid "PROT" and resid 47 and name HB2 ))
(( segid "PROT" and resid 47 and name HB1 ))
2.300 1.300 1.300 peak 5992 weight 0.10000E+01 volume 0.69282E+01 ppm1 2.844 ppm2 3.243
ASSI { 6002}
(( segid "PROT" and resid 42 and name HA ))
(( segid "PROT" and resid 42 and name HG1 ))
2.500 1.600 1.600 peak 6002 weight 0.10000E+01 volume 0.40649E+01 ppm1 4.505 ppm2 2.362
ASSI { 6022}
(( segid "PROT" and resid 87 and name HA ))
(( segid "PROT" and resid 87 and name HG1 ))
2.600 1.700 1.700 peak 6022 weight 0.10000E+01 volume 0.35044E+01 ppm1 4.342 ppm2 2.440
ASSI { 6052}
(( segid "PROT" and resid 83 and name HG2%))
(( segid "PROT" and resid 87 and name HG1 ))
2.900 2.100 2.100 peak 6052 weight 0.10000E+01 volume 0.17805E+01 ppm1 1.341 ppm2 2.456
ASSI { 6072}
(( segid "PROT" and resid 68 and name HA ))
(( segid "PROT" and resid 68 and name HB2 ))
2.900 2.100 2.100 peak 6072 weight 0.10000E+01 volume 0.17045E+01 ppm1 4.576 ppm2 2.958
ASSI { 6082}
(( segid "PROT" and resid 94 and name HA ))
(( segid "PROT" and resid 94 and name HG1 ))
2.200 1.200 1.200 peak 6082 weight 0.10000E+01 volume 0.84120E+01 ppm1 4.252 ppm2 2.257
ASSI { 6092}
(( segid "PROT" and resid 61 and name HA ))
(( segid "PROT" and resid 61 and name HG1 ))
2.500 1.600 1.600 peak 6092 weight 0.10000E+01 volume 0.40902E+01 ppm1 4.086 ppm2 2.414
ASSI { 6112}
(( segid "PROT" and resid 112 and name HA ))
(( segid "PROT" and resid 112 and name HG1 ))
2.600 1.700 1.700 peak 6112 weight 0.10000E+01 volume 0.34812E+01 ppm1 4.024 ppm2 2.394
ASSI { 6122}
(( segid "PROT" and resid 112 and name HA ))
(( segid "PROT" and resid 112 and name HG2 ))
2.600 1.700 1.700 peak 6122 weight 0.10000E+01 volume 0.35539E+01 ppm1 4.024 ppm2 2.252
ASSI { 6132}
(( segid "PROT" and resid 68 and name HB1 ))
(( segid "PROT" and resid 68 and name HB2 ))
2.400 1.400 1.400 peak 6132 weight 0.10000E+01 volume 0.51026E+01 ppm1 3.099 ppm2 2.959
ASSI { 6152}
(( segid "PROT" and resid 74 and name HB2 ))
(( segid "PROT" and resid 68 and name HB1 ))
2.800 2.000 2.000 peak 6152 weight 0.10000E+01 volume 0.19665E+01 ppm1 2.416 ppm2 3.093
ASSI { 6162}
(( segid "PROT" and resid 61 and name HB2 ))
(( segid "PROT" and resid 61 and name HG1 ))
1.800 0.800 0.800 peak 6162 weight 0.10000E+01 volume 0.28485E+02 ppm1 2.116 ppm2 2.409
ASSI { 6212}
(( segid "PROT" and resid 36 and name HA ))
(( segid "PROT" and resid 36 and name HG1 ))
2.800 2.000 2.000 peak 6212 weight 0.10000E+01 volume 0.23202E+01 ppm1 4.870 ppm2 2.207
ASSI { 6222}
(( segid "PROT" and resid 7 and name HA ))
(( segid "PROT" and resid 7 and name HG1 ))
2.800 2.000 2.000 peak 6222 weight 0.10000E+01 volume 0.19256E+01 ppm1 4.584 ppm2 2.309
ASSI { 6232}
(( segid "PROT" and resid 108 and name HA ))
(( segid "PROT" and resid 112 and name HG1 ))
2.400 1.400 1.400 peak 6232 weight 0.10000E+01 volume 0.59666E+01 ppm1 4.231 ppm2 2.438
ASSI { 6242}
(( segid "PROT" and resid 8 and name HD2 ))
(( segid "PROT" and resid 7 and name HG1 ))
2.900 2.100 2.100 peak 6242 weight 0.10000E+01 volume 0.17750E+01 ppm1 3.735 ppm2 2.302
ASSI { 6252}
(( segid "PROT" and resid 37 and name HD1 ))
(( segid "PROT" and resid 36 and name HG1 ))
2.700 1.800 1.800 peak 6252 weight 0.10000E+01 volume 0.27081E+01 ppm1 3.706 ppm2 2.205
ASSI { 6262}
(( segid "PROT" and resid 7 and name HB2 ))
(( segid "PROT" and resid 7 and name HG1 ))
2.200 1.200 1.200 peak 6262 weight 0.10000E+01 volume 0.10332E+02 ppm1 1.946 ppm2 2.303
ASSI { 6272}
(( segid "PROT" and resid 36 and name HB1 ))
(( segid "PROT" and resid 36 and name HG1 ))
2.100 1.100 1.100 peak 6272 weight 0.10000E+01 volume 0.12608E+02 ppm1 1.808 ppm2 2.210
ASSI { 6282}
(( segid "PROT" and resid 24 and name HA ))

```

```

(( segid "PROT" and resid 24 and name HG1 ))
2.500 1.600 1.600 peak 6282 weight 0.10000E+01 volume 0.40773E+01 ppm1 4 220 ppm2 2.889
ASSI { 6292}
(( segid "PROT" and resid 24 and name HA ))
(( segid "PROT" and resid 24 and name HG2 ))
2.300 1.300 1.300 peak 6292 weight 0.10000E+01 volume 0.62451E+01 ppm1 4.222 ppm2 2.498
ASSI { 6302}
(( segid "PROT" and resid 79 and name HA ))
(( segid "PROT" and resid 79 and name HG1 ))
2.400 1.400 1.400 peak 6302 weight 0.10000E+01 volume 0.53286E+01 ppm1 3.858 ppm2 2.467
ASSI { 6322}
(( segid "PROT" and resid 24 and name HG2 ))
(( segid "PROT" and resid 24 and name HG1 ))
1.900 0.900 0.900 peak 6322 weight 0.10000E+01 volume 0.19215E+02 ppm1 2.505 ppm2 2.890
ASSI { 6332}
(( segid "PROT" and resid 83 and name HG2 ))
(( segid "PROT" and resid 79 and name HG1 ))
2.800 2.000 2.000 peak 6332 weight 0.10000E+01 volume 0.22432E+01 ppm1 1.343 ppm2 2.481
ASSI { 6372}
(( segid "PROT" and resid 13 and name HA ))
(( segid "PROT" and resid 13 and name HG1 ))
2.500 1.600 1.600 peak 6372 weight 0.10000E+01 volume 0.38637E+01 ppm1 4.222 ppm2 2.535
ASSI { 6392}
(( segid "PROT" and resid 23 and name HA ))
(( segid "PROT" and resid 23 and name HG1 ))
2.500 1.600 1.600 peak 6392 weight 0.10000E+01 volume 0.39163E+01 ppm1 4.065 ppm2 2.594
ASSI { 6402}
(( segid "PROT" and resid 23 and name HA ))
(( segid "PROT" and resid 23 and name HG2 ))
2.500 1.600 1.600 peak 6402 weight 0.10000E+01 volume 0.41947E+01 ppm1 4.065 ppm2 2.484
ASSI { 6412}
(( segid "PROT" and resid 10 and name HB1 ))
(( segid "PROT" and resid 13 and name HG1 ))
3.000 2.200 2.200 peak 6412 weight 0.10000E+01 volume 0.15094E+01 ppm1 2.806 ppm2 2.528
ASSI { 6422}
(( segid "PROT" and resid 10 and name HB1 ))
(( segid "PROT" and resid 13 and name HG2 ))
2.800 2.000 2.000 peak 6422 weight 0.10000E+01 volume 0.20457E+01 ppm1 2.797 ppm2 2.417
ASSI { 6432}
(( segid "PROT" and resid 23 and name HB1 ))
(( segid "PROT" and resid 23 and name HG1 ))
2.100 1.100 1.100 peak 6432 weight 0.10000E+01 volume 0.10562E+02 ppm1 2.372 ppm2 2.598
ASSI { 6442}
(( segid "PROT" and resid 23 and name HB2 ))
(( segid "PROT" and resid 23 and name HG1 ))
2.300 1.300 1.300 peak 6442 weight 0.10000E+01 volume 0.70727E+01 ppm1 2.270 ppm2 2.591
ASSI { 6472}
(( segid "PROT" and resid 49 and name HG1 ))
(( segid "PROT" and resid 49 and name HB ))
2.300 1.300 1.300 peak 6472 weight 0.10000E+01 volume 0.67655E+01 ppm1 0.964 ppm2 1.928
ASSI { 6492}
(( segid "PROT" and resid 60 and name HA ))
(( segid "PROT" and resid 59 and name HB2 ))
2.400 2.400 2.100 peak 6492 weight 0.10000E+01 volume 0.56526E+01 ppm1 4.451 ppm2 1.936
ASSI { 6582}
(( segid "PROT" and resid 75 and name HB1 ))
(( segid "PROT" and resid 75 and name HB2 ))
2.100 1.100 1.100 peak 6582 weight 0.10000E+01 volume 0.12724E+02 ppm1 2.964 ppm2 2.649
ASSI { 6602}
(( segid "PROT" and resid 112 and name HG2 ))
(( segid "PROT" and resid 111 and name HB1 ))
2.400 1.400 1.400 peak 6602 weight 0.10000E+01 volume 0.55476E+01 ppm1 2.218 ppm2 1.930
ASSI { 6622}
(( segid "PROT" and resid 75 and name HE ))
(( segid "PROT" and resid 75 and name HB2 ))
2.600 1.700 1.700 peak 6622 weight 0.10000E+01 volume 0.29895E+01 ppm1 2.095 ppm2 2.645
ASSI { 6702}
(( segid "PROT" and resid 53 and name HA ))
(( segid "PROT" and resid 53 and name HB1 ))
2.200 1.200 1.200 peak 6702 weight 0.10000E+01 volume 0.84112E+01 ppm1 4.123 ppm2 2.249
ASSI { 6722}
(( segid "PROT" and resid 16 and name HB2 ))
(( segid "PROT" and resid 19 and name HB1 ))
2.600 1.700 1.700 peak 6722 weight 0.10000E+01 volume 0.32944E+01 ppm1 3.944 ppm2 1.738
ASSI { 6732}
(( segid "PROT" and resid 16 and name HB2 ))
(( segid "PROT" and resid 19 and name HB2 ))
2.800 2.000 2.000 peak 6732 weight 0.10000E+01 volume 0.19396E+01 ppm1 3.944 ppm2 1.404
ASSI { 6742}
(( segid "PROT" and resid 11 and name HD1 ))
(( segid "PROT" and resid 11 and name HB1 ))
2.500 1.600 1.600 peak 6742 weight 0.10000E+01 volume 0.38499E+01 ppm1 3.937 ppm2 2.367
ASSI { 6802}
(( segid "PROT" and resid 19 and name HD1 ))
(( segid "PROT" and resid 19 and name HB2 ))
2.700 1.800 1.800 peak 6802 weight 0.10000E+01 volume 0.24759E+01 ppm1 1.636 ppm2 1.405
ASSI { 6822}
(( segid "PROT" and resid 104 and name HG1 ))
(( segid "PROT" and resid 104 and name HB1 ))

```



```

ASSI { 7262}
  (( segid "PROT" and resid 91 and name HG1 ))
  (( segid "PROT" and resid 91 and name HB1 ))
  2.400 1.400 1.400 peak 7262 weight 0.10000E+01 volume 0.59619E+01 ppm1 1.990 ppm2 1.628
ASSI { 7302}
  (( segid "PROT" and resid 109 and name HG1 ))
  (( segid "PROT" and resid 109 and name HB2 ))
  2.600 1.700 1.700 peak 7302 weight 0.10000E+01 volume 0.36664E+01 ppm1 0.853 ppm2 1.586
ASSI { 7312}
  (( segid "PROT" and resid 36 and name HA ))
  (( segid "PROT" and resid 36 and name HB1 ))
  2.900 2.100 2.100 peak 7312 weight 0.10000E+01 volume 0.17361E+01 ppm1 4.873 ppm2 2.145
ASSI { 7322}
  (( segid "PROT" and resid 36 and name HA ))
  (( segid "PROT" and resid 36 and name HB2 ))
  2.900 2.100 2.100 peak 7322 weight 0.10000E+01 volume 0.18767E+01 ppm1 4.866 ppm2 1.802
ASSI { 7332}
  (( segid "PROT" and resid 69 and name HA ))
  (( segid "PROT" and resid 69 and name HB ))
  2.100 1.100 1.100 peak 7332 weight 0.10000E+01 volume 0.11082E+02 ppm1 4.121 ppm2 2 350
ASSI { 7342}
  (( segid "PROT" and resid 36 and name HG1 ))
  (( segid "PROT" and resid 36 and name HB2 ))
  2.000 1.000 1.000 peak 7342 weight 0.10000E+01 volume 0.14522E+02 ppm1 2.193 ppm2 1.800
ASSI { 7352}
  (( segid "PROT" and resid 36 and name HB2 ))
  (( segid "PROT" and resid 36 and name HB1 ))
  2.000 1.000 1.000 peak 7352 weight 0.10000E+01 volume 0.13927E+02 ppm1 1.804 ppm2 2.149
ASSI { 7392}
  (( segid "PROT" and resid 54 and name HG1 ))
  (( segid "PROT" and resid 54 and name HB2 ))
  2.900 2.100 2.100 peak 7392 weight 0.10000E+01 volume 0.16439E+01 ppm1 2.747 ppm2 1.390
ASSI { 7402}
  (( segid "PROT" and resid 54 and name HG1 ))
  (( segid "PROT" and resid 54 and name HB1 ))
  2.900 2.100 2.100 peak 7402 weight 0.10000E+01 volume 0.16583E+01 ppm1 2.739 ppm2 2.035
ASSI { 7412}
  (( segid "PROT" and resid 90 and name HB1 ))
  (( segid "PROT" and resid 90 and name HB2 ))
  2.100 1.100 1.100 peak 7412 weight 0.10000E+01 volume 0.12123E+02 ppm1 2.347 ppm2 2.182
ASSI { 7422}
  (( segid "PROT" and resid 54 and name HB1 ))
  (( segid "PROT" and resid 54 and name HB2 ))
  2.600 1.700 1.700 peak 7422 weight 0.10000E+01 volume 0.35394E+01 ppm1 2.028 ppm2 1.380
ASSI { 7452}
  (( segid "PROT" and resid 42 and name HA ))
  (( segid "PROT" and resid 42 and name HB2 ))
  2.600 1.700 1.700 peak 7452 weight 0.10000E+01 volume 0.33452E+01 ppm1 4.508 ppm2 2.075
ASSI { 7462}
  (( segid "PROT" and resid 9 and name HA ))
  (( segid "PROT" and resid 9 and name HB1 ))
  2.300 1.300 1.300 peak 7462 weight 0.10000E+01 volume 0.64998E+01 ppm1 4.364 ppm2 1.873
ASSI { 7492}
  (( segid "PROT" and resid 81 and name HA ))
  (( segid "PROT" and resid 81 and name HB ))
  2.700 1.800 1.800 peak 7492 weight 0.10000E+01 volume 0.25831E+01 ppm1 3.126 ppm2 1.465
ASSI { 7502}
  (( segid "PROT" and resid 54 and name HG1 ))
  (( segid "PROT" and resid 54 and name HG2 ))
  2.600 1.700 1.700 peak 7502 weight 0.10000E+01 volume 0.36087E+01 ppm1 2.746 ppm2 1.897
ASSI { 7532}
  (( segid "PROT" and resid 81 and name HG1 ))
  (( segid "PROT" and resid 54 and name HG2 ))
  2.800 2.000 2.000 peak 7532 weight 0.10000E+01 volume 0.21318E+01 ppm1 0.508 ppm2 1.898
ASSI { 7602}
  (( segid "PROT" and resid 51 and name HD1 ))
  (( segid "PROT" and resid 51 and name HB2 ))
  2.700 1.800 1.800 peak 7602 weight 0.10000E+01 volume 0.27404E+01 ppm1 3.022 ppm2 1.212
ASSI { 7612}
  (( segid "PROT" and resid 57 and name HE2 ))
  (( segid "PROT" and resid 57 and name HB2 ))
  2.600 1.700 1.700 peak 7612 weight 0.10000E+01 volume 0.31496E+01 ppm1 2.081 ppm2 1.144
ASSI { 7632}
  (( segid "PROT" and resid 51 and name HB2 ))
  (( segid "PROT" and resid 51 and name HB1 ))
  1.900 0.900 0.900 peak 7632 weight 0.10000E+01 volume 0.23953E+02 ppm1 1.213 ppm2 1.384
ASSI { 7652}
  (( segid "PROT" and resid 87 and name HA ))
  (( segid "PROT" and resid 87 and name HB1 ))
  2.200 1.200 1.200 peak 7652 weight 0.10000E+01 volume 0.80014E+01 ppm1 4.343 ppm2 2.226
ASSI { 7662}
  (( segid "PROT" and resid 87 and name HA ))
  (( segid "PROT" and resid 87 and name HB2 ))
  2.200 1.200 1.200 peak 7662 weight 0.10000E+01 volume 0.87899E+01 ppm1 4.341 ppm2 2.060
ASSI { 7682}
  (( segid "PROT" and resid 87 and name HG2 ))
  (( segid "PROT" and resid 87 and name HB2 ))
  1.700 0.700 0.700 peak 7682 weight 0.10000E+01 volume 0.37037E+02 ppm1 2.240 ppm2 2.075
ASSI { 7692}

```



```

{ segid "PROT" and resid 113 and name HB1 }
(( segid "PROT" and resid 112 and name HB1 ))
2.500 1.600 1.600 peak 7692 weight 0.10000E+01 volume 0.37285E+01 ppm1 1.414 ppm2 2.097
ASSI { 7702}
(( segid "PROT" and resid 33 and name HB1 ))
(( segid "PROT" and resid 33 and name HB2 ))
3.000 2.200 2.200 peak 7702 weight 0.10000E+01 volume 0.15063E+01 ppm1 1.078 ppm2 -0.431
ASSI { 7712}
{ segid "PROT" and resid 49 and name HG2 }
(( segid "PROT" and resid 87 and name HB2 ))
2.900 2.100 2.100 peak 7712 weight 0.10000E+01 volume 0.15587E+01 ppm1 0.905 ppm2 2.080
ASSI { 7762}
(( segid "PROT" and resid 104 and name HA ))
(( segid "PROT" and resid 103 and name HG2 ))
2.200 1.200 1.200 peak 7762 weight 0.10000E+01 volume 0.86935E+01 ppm1 4.098 ppm2 1.957
ASSI { 7772}
(( segid "PROT" and resid 112 and name HA ))
(( segid "PROT" and resid 112 and name HB1 ))
2.000 1.000 1.000 peak 7772 weight 0.10000E+01 volume 0.14908E+02 ppm1 4.024 ppm2 2.107
ASSI { 7832}
(( segid "PROT" and resid 103 and name HG2 ))
(( segid "PROT" and resid 103 and name HB2 ))
2.500 1.600 1.600 peak 7832 weight 0.10000E+01 volume 0.43617E+01 ppm1 1.952 ppm2 1.324
ASSI { 7842}
(( segid "PROT" and resid 103 and name HB1 ))
(( segid "PROT" and resid 103 and name HB2 ))
2.100 1.100 1.100 peak 7842 weight 0.10000E+01 volume 0.10363E+02 ppm1 1.792 ppm2 1.333
ASSI { 7902}
(( segid "PROT" and resid 7 and name HA ))
(( segid "PROT" and resid 7 and name HB1 ))
2.700 1.800 1.800 peak 7902 weight 0.10000E+01 volume 0.24043E+01 ppm1 4.586 ppm2 2.070
ASSI { 7912}
(( segid "PROT" and resid 7 and name HA ))
(( segid "PROT" and resid 7 and name HB2 ))
2.800 2.000 2.000 peak 7912 weight 0.10000E+01 volume 0.21766E+01 ppm1 4.585 ppm2 1.943
ASSI { 7942}
(( segid "PROT" and resid 24 and name HA ))
(( segid "PROT" and resid 24 and name HB1 ))
2.600 1.700 1.700 peak 7942 weight 0.10000E+01 volume 0.31104E+01 ppm1 4.221 ppm2 2.495
ASSI { 7972}
(( segid "PROT" and resid 8 and name HD2 ))
(( segid "PROT" and resid 7 and name HB1 ))
2.900 2.100 2.100 peak 7972 weight 0.10000E+01 volume 0.17393E+01 ppm1 3.717 ppm2 2.078
ASSI { 7992}
(( segid "PROT" and resid 111 and name HE1 ))
(( segid "PROT" and resid 111 and name HD1 ))
2.100 1.100 1.100 peak 7992 weight 0.10000E+01 volume 0.13020E+02 ppm1 2.959 ppm2 1.646
ASSI { 8002}
(( segid "PROT" and resid 24 and name HG1 ))
(( segid "PROT" and resid 24 and name HB1 ))
2.500 1.600 1.600 peak 8002 weight 0.10000E+01 volume 0.39707E+01 ppm1 2.890 ppm2 2.505
ASSI { 8022}
(( segid "PROT" and resid 24 and name HG2 ))
(( segid "PROT" and resid 24 and name HB2 ))
2.200 1.200 1.200 peak 8022 weight 0.10000E+01 volume 0.10130E+02 ppm1 2.510 ppm2 2.415
ASSI { 8042}
(( segid "PROT" and resid 24 and name HB2 ))
(( segid "PROT" and resid 24 and name HB1 ))
2.400 1.400 1.400 peak 8042 weight 0.10000E+01 volume 0.59198E+01 ppm1 2.416 ppm2 2.519
ASSI { 8052}
(( segid "PROT" and resid 112 and name HG1 ))
(( segid "PROT" and resid 112 and name HB1 ))
1.800 0.800 0.800 peak 8052 weight 0.10000E+01 volume 0.25596E+02 ppm1 2.396 ppm2 2.120
ASSI { 8082}
(( segid "PROT" and resid 111 and name HG2 ))
(( segid "PROT" and resid 111 and name HD1 ))
2.000 1.000 1.000 peak 8082 weight 0.10000E+01 volume 0.17175E+02 ppm1 1.323 ppm2 1.639
ASSI { 8092}
{ segid "PROT" and resid 63 and name HD1 }
(( segid "PROT" and resid 19 and name HD1 ))
2.700 1.800 1.800 peak 8092 weight 0.10000E+01 volume 0.28800E+01 ppm1 0.916 ppm2 1.647
ASSI { 8112}
(( segid "PROT" and resid 64 and name HA ))
(( segid "PROT" and resid 64 and name HD1 ))
2.600 1.700 1.700 peak 8112 weight 0.10000E+01 volume 0.36099E+01 ppm1 4.372 ppm2 1.788
ASSI { 8142}
(( segid "PROT" and resid 80 and name HD1 ))
(( segid "PROT" and resid 80 and name HB2 ))
2.900 2.100 2.100 peak 8142 weight 0.10000E+01 volume 0.16213E+01 ppm1 3.407 ppm2 1.957
ASSI { 8172}
(( segid "PROT" and resid 61 and name HG2 ))
(( segid "PROT" and resid 57 and name HE2 ))
1.700 1.700 2.800 peak 8172 weight 0.10000E+01 volume 0.41822E+02 ppm1 2.258 ppm2 2.109
ASSI { 8192}
(( segid "PROT" and resid 101 and name HG1 ))
(( segid "PROT" and resid 101 and name HG12 ))
2.100 1.100 1.100 peak 8192 weight 0.10000E+01 volume 0.11529E+02 ppm1 1.893 ppm2 1.242
ASSI { 8252}
{ segid "PROT" and resid 104 and name HA }

```

```

(( segid "PROT" and resid 104 and name HD1 ))
2.300 1.300 1.300 peak 8252 weight 0.10000E+01 volume 0.66354E+01 ppm1 4.101 ppm2 1.755
ASSI { 8272}
(( segid "PROT" and resid 104 and name HE1 ))
(( segid "PROT" and resid 104 and name HD1 ))
1.800 0.800 0.800 peak 8272 weight 0.10000E+01 volume 0.33570E+02 ppm1 3.023 ppm2 1.747
ASSI { 8282}
(( segid "PROT" and resid 57 and name HE2 ))
(( segid "PROT" and resid 57 and name HD2 ))
2.800 2.000 2.000 peak 8282 weight 0.10000E+01 volume 0.22756E+01 ppm1 2.085 ppm2 0.913
ASSI { 8292}
(( segid "PROT" and resid 104 and name HB1 ))
(( segid "PROT" and resid 104 and name HD1 ))
2.000 1.000 1.000 peak 8292 weight 0.10000E+01 volume 0.18472E+02 ppm1 1.961 ppm2 1.747
ASSI { 8312}
(( segid "PROT" and resid 104 and name HG1 ))
(( segid "PROT" and resid 104 and name HD1 ))
1.700 1.700 2.800 peak 8312 weight 0.10000E+01 volume 0.40675E+02 ppm1 1.554 ppm2 1.741
ASSI { 8322}
(( segid "PROT" and resid 104 and name HG2 ))
(( segid "PROT" and resid 104 and name HD1 ))
1.600 1.600 2.900 peak 8322 weight 0.10000E+01 volume 0.59831E+02 ppm1 1.468 ppm2 1.706
ASSI { 8332}
(( segid "PROT" and resid 57 and name HD2 ))
(( segid "PROT" and resid 57 and name HD1 ))
2.600 1.700 1.700 peak 8332 weight 0.10000E+01 volume 0.35657E+01 ppm1 0.915 ppm2 1.760
ASSI { 8342}
(( segid "PROT" and resid 61 and name HA ))
(( segid "PROT" and resid 61 and name HB1 ))
2.300 1.300 1.300 peak 8342 weight 0.10000E+01 volume 0.77843E+01 ppm1 4.093 ppm2 2.248
ASSI { 8352}
(( segid "PROT" and resid 79 and name HA ))
(( segid "PROT" and resid 79 and name HB1 ))
2.300 1.300 1.300 peak 8352 weight 0.10000E+01 volume 0.66007E+01 ppm1 3.864 ppm2 2.222
ASSI { 8362}
(( segid "PROT" and resid 79 and name HA ))
(( segid "PROT" and resid 79 and name HB2 ))
2.300 1.300 1.300 peak 8362 weight 0.10000E+01 volume 0.61698E+01 ppm1 3.862 ppm2 2.112
ASSI { 8372}
(( segid "PROT" and resid 94 and name HA ))
(( segid "PROT" and resid 94 and name HB1 ))
1.900 0.900 0.900 peak 8372 weight 0.10000E+01 volume 0.24388E+02 ppm1 4.244 ppm2 2.144
ASSI { 8382}
(( segid "PROT" and resid 10 and name HB1 ))
(( segid "PROT" and resid 13 and name HB1 ))
2.600 1.700 1.700 peak 8382 weight 0.10000E+01 volume 0.29895E+01 ppm1 2.798 ppm2 2.191
ASSI { 8392}
(( segid "PROT" and resid 13 and name HG1 ))
(( segid "PROT" and resid 13 and name HB1 ))
2.000 1.000 1.000 peak 8392 weight 0.10000E+01 volume 0.13858E+02 ppm1 2.536 ppm2 2.194
ASSI { 8402}
(( segid "PROT" and resid 13 and name HG2 ))
(( segid "PROT" and resid 13 and name HB1 ))
1.800 0.800 0.800 peak 8402 weight 0.10000E+01 volume 0.32827E+02 ppm1 2.431 ppm2 2.183
ASSI { 8472}
(( segid "PROT" and resid 106 and name HB2 ))
(( segid "PROT" and resid 21 and name HG11))
2.400 2.400 2.100 peak 8472 weight 0.10000E+01 volume 0.49094E+01 ppm1 3.161 ppm2 1.823
ASSI { 8482}
(( segid "PROT" and resid 21 and name HB ))
(( segid "PROT" and resid 21 and name HG11))
2.000 1.000 1.000 peak 8482 weight 0.10000E+01 volume 0.13836E+02 ppm1 1.954 ppm2 1.787
ASSI { 8512}
(( segid "PROT" and resid 21 and name HG12))
(( segid "PROT" and resid 21 and name HG11))
2.100 1.100 1.100 peak 8512 weight 0.10000E+01 volume 0.11436E+02 ppm1 1.070 ppm2 1.790
ASSI { 8542}
(( segid "PROT" and resid 20 and name HA ))
(( segid "PROT" and resid 23 and name HB1 ))
2.600 1.700 1.700 peak 8542 weight 0.10000E+01 volume 0.33979E+01 ppm1 4.328 ppm2 2.370
ASSI { 8552}
(( segid "PROT" and resid 20 and name HA ))
(( segid "PROT" and resid 23 and name HB2 ))
2.600 1.700 1.700 peak 8552 weight 0.10000E+01 volume 0.34588E+01 ppm1 4.325 ppm2 2.260
ASSI { 8562}
(( segid "PROT" and resid 23 and name HA ))
(( segid "PROT" and resid 23 and name HB1 ))
2.300 1.300 1.300 peak 8562 weight 0.10000E+01 volume 0.72048E+01 ppm1 4.066 ppm2 2.368
ASSI { 8592}
(( segid "PROT" and resid 23 and name HG2 ))
(( segid "PROT" and resid 23 and name HB1 ))
2.300 1.300 1.300 peak 8592 weight 0.10000E+01 volume 0.65153E+01 ppm1 2.490 ppm2 2.359
ASSI { 8602}
(( segid "PROT" and resid 23 and name HB1 ))
(( segid "PROT" and resid 23 and name HB2 ))
1.900 0.900 0.900 peak 8602 weight 0.10000E+01 volume 0.20845E+02 ppm1 2.371 ppm2 2.263
ASSI { 8652}
(( segid "PROT" and resid 53 and name HA ))
(( segid "PROT" and resid 53 and name HG2 ))

```

2.800	2.000	2.000	peak	8652	weight	0.10000E+01	volume	0.23066E+01	ppm1	4.123	ppm2	1.937
ASSI { 8682}												
((segid "PROT" and resid 32 and name HB1))												
((segid "PROT" and resid 32 and name HB2))												
2.400	1.400	1.400	peak	8682	weight	0.10000E+01	volume	0.48514E+01	ppm1	3.640	ppm2	3.407
ASSI { 8712}												
((segid "PROT" and resid 53 and name HG1))												
((segid "PROT" and resid 53 and name HG2))												
2.000	1.000	1.000	peak	8712	weight	0.10000E+01	volume	0.17544E+02	ppm1	2.274	ppm2	1.953
ASSI { 8752}												
((segid "PROT" and resid 44 and name HA))												
((segid "PROT" and resid 44 and name HG2))												
2.600	1.700	1.700	peak	8752	weight	0.10000E+01	volume	0.31327E+01	ppm1	4.552	ppm2	2.078
ASSI { 8762}												
((segid "PROT" and resid 44 and name HA))												
((segid "PROT" and resid 44 and name HG1))												
2.900	2.100	2.100	peak	8762	weight	0.10000E+01	volume	0.18869E+01	ppm1	4.546	ppm2	2.204
ASSI { 8772}												
((segid "PROT" and resid 66 and name HA))												
((segid "PROT" and resid 66 and name HG1))												
2.600	1.700	1.700	peak	8772	weight	0.10000E+01	volume	0.35462E+01	ppm1	4.442	ppm2	1.614
ASSI { 8792}												
((segid "PROT" and resid 44 and name HD2))												
((segid "PROT" and resid 44 and name HG2))												
2.600	1.700	1.700	peak	8792	weight	0.10000E+01	volume	0.37158E+01	ppm1	3.569	ppm2	2.086
ASSI { 8812}												
((segid "PROT" and resid 66 and name HD1))												
((segid "PROT" and resid 66 and name HG1))												
2.500	1.600	1.600	peak	8812	weight	0.10000E+01	volume	0.43300E+01	ppm1	3.103	ppm2	1.614
ASSI { 8822}												
((segid "PROT" and resid 66 and name HB1))												
((segid "PROT" and resid 66 and name HG2))												
2.300	1.300	1.300	peak	8822	weight	0.10000E+01	volume	0.67305E+01	ppm1	2.133	ppm2	1.573
ASSI { 8832}												
((segid "PROT" and resid 66 and name HB2))												
((segid "PROT" and resid 66 and name HG2))												
2.400	1.400	1.400	peak	8832	weight	0.10000E+01	volume	0.56248E+01	ppm1	2.050	ppm2	1.575
ASSI { 8862}												
((segid "PROT" and resid 78 and name HB2))												
((segid "PROT" and resid 78 and name HG))												
2.400	1.400	1.400	peak	8862	weight	0.10000E+01	volume	0.56132E+01	ppm1	0.474	ppm2	0.694
ASSI { 8892}												
((segid "PROT" and resid 10 and name HA))												
((segid "PROT" and resid 11 and name HG1))												
2.900	2.100	2.100	peak	8892	weight	0.10000E+01	volume	0.15699E+01	ppm1	4.919	ppm2	2.106
ASSI { 8902}												
((segid "PROT" and resid 8 and name HA))												
((segid "PROT" and resid 8 and name HG1))												
2.500	1.600	1.600	peak	8902	weight	0.10000E+01	volume	0.38281E+01	ppm1	4.463	ppm2	2.061
ASSI { 8912}												
((segid "PROT" and resid 11 and name HA))												
((segid "PROT" and resid 11 and name HG1))												
2.500	1.600	1.600	peak	8912	weight	0.10000E+01	volume	0.41483E+01	ppm1	4.376	ppm2	2.096
ASSI { 8932}												
((segid "PROT" and resid 11 and name HD1))												
((segid "PROT" and resid 11 and name HG1))												
2.000	1.000	1.000	peak	8932	weight	0.10000E+01	volume	0.15330E+02	ppm1	3.902	ppm2	2.097
ASSI { 8962}												
((segid "PROT" and resid 91 and name HA))												
((segid "PROT" and resid 91 and name HG2))												
2.800	2.000	2.000	peak	8962	weight	0.10000E+01	volume	0.19450E+01	ppm1	2.589	ppm2	1.708
ASSI { 8972}												
((segid "PROT" and resid 11 and name HB1))												
((segid "PROT" and resid 11 and name HG1))												
2.000	1.000	1.000	peak	8972	weight	0.10000E+01	volume	0.17135E+02	ppm1	2.382	ppm2	2.098
ASSI { 8982}												
((segid "PROT" and resid 8 and name HB1))												
((segid "PROT" and resid 8 and name HG1))												
1.800	0.800	0.800	peak	8982	weight	0.10000E+01	volume	0.27927E+02	ppm1	2.290	ppm2	2.056
ASSI { 8992}												
((segid "PROT" and resid 8 and name HB2))												
((segid "PROT" and resid 8 and name HG1))												
2.100	1.100	1.100	peak	8992	weight	0.10000E+01	volume	0.11694E+02	ppm1	1.923	ppm2	2.056
ASSI { 9002}												
((segid "PROT" and resid 91 and name HG2))												
((segid "PROT" and resid 91 and name HG1))												
2.000	1.000	1.000	peak	9002	weight	0.10000E+01	volume	0.16829E+02	ppm1	1.710	ppm2	1.994
ASSI { 9022}												
((segid "PROT" and resid 73 and name HD1%))												
((segid "PROT" and resid 73 and name HG))												
2.100	1.100	1.100	peak	9022	weight	0.10000E+01	volume	0.10664E+02	ppm1	0.971	ppm2	1.797
ASSI { 9032}												
((segid "PROT" and resid 73 and name HD2%))												
((segid "PROT" and resid 73 and name HG))												
2.100	1.100	1.100	peak	9032	weight	0.10000E+01	volume	0.10796E+02	ppm1	0.932	ppm2	1.808
ASSI { 9042}												
((segid "PROT" and resid 14 and name HD2%))												
((segid "PROT" and resid 8 and name HG1))												
2.800	2.000	2.000	peak	9042	weight	0.10000E+01	volume	0.20174E+01	ppm1	0.832	ppm2	2.058

```

ASSI { 9062}
  (( segid "PROT" and resid 9 and name HA ))
  (( segid "PROT" and resid 9 and name HG1 ))
  2.500 1.600 1.600 peak 9062 weight 0.10000E+01 volume 0.42875E+01 ppm1 4.362 ppm2 1.682
ASSI { 9072}
  (( segid "PROT" and resid 115 and name HA ))
  (( segid "PROT" and resid 115 and name HG ))
  2.700 1.800 1.800 peak 9072 weight 0.10000E+01 volume 0.26718E+01 ppm1 4.257 ppm2 1.567
ASSI { 9092}
  (( segid "PROT" and resid 9 and name HD1 ))
  (( segid "PROT" and resid 9 and name HG1 ))
  2.300 1.300 1.300 peak 9092 weight 0.10000E+01 volume 0.71572E+01 ppm1 3.224 ppm2 1.693
ASSI { 9122}
  (( segid "PROT" and resid 22 and name HB1 ))
  (( segid "PROT" and resid 22 and name HG ))
  2.300 1.300 1.300 peak 9122 weight 0.10000E+01 volume 0.64668E+01 ppm1 2.122 ppm2 1.784
ASSI { 9132}
  (( segid "PROT" and resid 80 and name HB1 ))
  (( segid "PROT" and resid 80 and name HG1 ))
  1.900 0.900 0.900 peak 9132 weight 0.10000E+01 volume 0.21048E+02 ppm1 2.009 ppm2 1.780
ASSI { 9142}
  (( segid "PROT" and resid 9 and name HB1 ))
  (( segid "PROT" and resid 9 and name HG1 ))
  1.900 0.900 0.900 peak 9142 weight 0.10000E+01 volume 0.23404E+02 ppm1 1.864 ppm2 1.689
ASSI { 9152}
  (( segid "PROT" and resid 37 and name HB2 ))
  (( segid "PROT" and resid 37 and name HG1 ))
  2.500 1.600 1.600 peak 9152 weight 0.10000E+01 volume 0.37817E+01 ppm1 1.704 ppm2 2.175
ASSI { 9172}
  (( segid "PROT" and resid 115 and name HD1% ))
  (( segid "PROT" and resid 115 and name HG ))
  2.000 1.000 1.000 peak 9172 weight 0.10000E+01 volume 0.15406E+02 ppm1 0.766 ppm2 1.571
ASSI { 9192}
  (( segid "PROT" and resid 110 and name HG2% ))
  (( segid "PROT" and resid 115 and name HG ))
  2.900 2.100 2.100 peak 9192 weight 0.10000E+01 volume 0.16502E+01 ppm1 0.684 ppm2 1.556
ASSI { 9202}
  (( segid "PROT" and resid 15 and name HE% ))
  (( segid "PROT" and resid 63 and name HD1% ))
  2.600 1.700 1.700 peak 9202 weight 0.10000E+01 volume 0.29945E+01 ppm1 6.925 ppm2 0.919
ASSI { 9212}
  (( segid "PROT" and resid 35 and name HA ))
  (( segid "PROT" and resid 56 and name HD1% ))
  2.700 1.800 1.800 peak 9212 weight 0.10000E+01 volume 0.25843E+01 ppm1 4.340 ppm2 0.976
ASSI { 9222}
  (( segid "PROT" and resid 116 and name HA ))
  (( segid "PROT" and resid 116 and name HG11 ))
  2.800 2.000 2.000 peak 9222 weight 0.10000E+01 volume 0.19299E+01 ppm1 4.274 ppm2 1.350
ASSI { 9232}
  (( segid "PROT" and resid 116 and name HA ))
  (( segid "PROT" and resid 116 and name HG12 ))
  2.700 1.800 1.800 peak 9232 weight 0.10000E+01 volume 0.25639E+01 ppm1 4.273 ppm2 0.964
ASSI { 9242}
  (( segid "PROT" and resid 56 and name HA ))
  (( segid "PROT" and resid 56 and name HD1% ))
  2.600 1.700 1.700 peak 9242 weight 0.10000E+01 volume 0.30591E+01 ppm1 4.078 ppm2 0.966
ASSI { 9272}
  (( segid "PROT" and resid 26 and name HA ))
  (( segid "PROT" and resid 56 and name HD1% ))
  2.500 1.600 1.600 peak 9272 weight 0.10000E+01 volume 0.37902E+01 ppm1 3.935 ppm2 0.976
ASSI { 9352}
  (( segid "PROT" and resid 34 and name HB2 ))
  (( segid "PROT" and resid 56 and name HD1% ))
  2.700 1.800 1.800 peak 9352 weight 0.10000E+01 volume 0.23627E+01 ppm1 2.636 ppm2 0.979
ASSI { 9382}
  (( segid "PROT" and resid 35 and name HE% ))
  (( segid "PROT" and resid 56 and name HD1% ))
  2.700 1.800 1.800 peak 9382 weight 0.10000E+01 volume 0.24784E+01 ppm1 2.218 ppm2 0.976
ASSI { 9392}
  (( segid "PROT" and resid 112 and name HB1 ))
  (( segid "PROT" and resid 109 and name HD1 ))
  2.700 1.800 1.800 peak 9392 weight 0.10000E+01 volume 0.25178E+01 ppm1 2.113 ppm2 1.417
ASSI { 9402}
  (( segid "PROT" and resid 56 and name HB1 ))
  (( segid "PROT" and resid 56 and name HD1% ))
  2.500 1.600 1.600 peak 9402 weight 0.10000E+01 volume 0.42717E+01 ppm1 2.108 ppm2 0.974
ASSI { 9422}
  (( segid "PROT" and resid 116 and name HB ))
  (( segid "PROT" and resid 116 and name HG11 ))
  2.400 1.400 1.400 peak 9422 weight 0.10000E+01 volume 0.48995E+01 ppm1 1.853 ppm2 1.353
ASSI { 9442}
  (( segid "PROT" and resid 56 and name HG ))
  (( segid "PROT" and resid 56 and name HD1% ))
  2.100 1.100 1.100 peak 9442 weight 0.10000E+01 volume 0.12057E+02 ppm1 1.763 ppm2 0.967
ASSI { 9462}
  (( segid "PROT" and resid 56 and name HB2 ))
  (( segid "PROT" and resid 56 and name HD1% ))
  2.500 1.600 1.600 peak 9462 weight 0.10000E+01 volume 0.42508E+01 ppm1 1.450 ppm2 0.967
ASSI { 9482}

```

```

(( segid "PROT" and resid 116 and name HG11))
(( segid "PROT" and resid 116 and name HG12))
1.900 0.900 0.900 peak 9482 weight 0.10000E+01 volume 0.19352E+02 ppm1 1.347 ppm2 0.964
ASSI { 9492}
(( segid "PROT" and resid 51 and name HB2 ))
(( segid "PROT" and resid 51 and name HG1 ))
1.900 0.900 0.900 peak 9492 weight 0.10000E+01 volume 0.20832E+02 ppm1 1.212 ppm2 1.350
ASSI { 9512}
(( segid "PROT" and resid 63 and name HD2%))
(( segid "PROT" and resid 63 and name HD1%))
1.900 0.900 0.900 peak 9512 weight 0.10000E+01 volume 0.20111E+02 ppm1 1.080 ppm2 0.919
ASSI { 9542}
(( segid "PROT" and resid 14 and name HD1%))
(( segid "PROT" and resid 14 and name HG ))
2.000 1.000 1.000 peak 9542 weight 0.10000E+01 volume 0.14691E+02 ppm1 0.846 ppm2 1.439
ASSI { 9582}
(( segid "PROT" and resid 34 and name HZ ))
(( segid "PROT" and resid 85 and name HB1 ))
2.700 1.800 1.800 peak 9582 weight 0.10000E+01 volume 0.27166E+01 ppm1 7.291 ppm2 3.407
ASSI { 9592}
(( segid "PROT" and resid 34 and name HZ ))
(( segid "PROT" and resid 85 and name HB2 ))
2.900 2.100 2.100 peak 9592 weight 0.10000E+01 volume 0.18097E+01 ppm1 7.295 ppm2 3.062
ASSI { 9602}
(( segid "PROT" and resid 82 and name HE% ))
(( segid "PROT" and resid 102 and name HG ))
2.800 2.000 2.000 peak 9602 weight 0.10000E+01 volume 0.23143E+01 ppm1 6.462 ppm2 1.600
ASSI { 9612}
(( segid "PROT" and resid 85 and name HA ))
(( segid "PROT" and resid 85 and name HB1 ))
2.700 1.800 1.800 peak 9612 weight 0.10000E+01 volume 0.25087E+01 ppm1 4.515 ppm2 3.415
ASSI { 9642}
(( segid "PROT" and resid 98 and name HA ))
(( segid "PROT" and resid 98 and name HB2 ))
2.700 1.800 1.800 peak 9642 weight 0.10000E+01 volume 0.24656E+01 ppm1 4.220 ppm2 3.078
ASSI { 9652}
(( segid "PROT" and resid 85 and name HB1 ))
(( segid "PROT" and resid 85 and name HB2 ))
2.200 1.200 1.200 peak 9652 weight 0.10000E+01 volume 0.83966E+01 ppm1 3.413 ppm2 3.084
ASSI { 9692}
(( segid "PROT" and resid 25 and name HG2%))
(( segid "PROT" and resid 102 and name HG ))
2.700 1.800 1.800 peak 9692 weight 0.10000E+01 volume 0.26216E+01 ppm1 1.068 ppm2 1.577
ASSI { 9712}
(( segid "PROT" and resid 60 and name HB1 ))
(( segid "PROT" and resid 22 and name HD1%))
2.300 1.300 1.300 peak 9712 weight 0.10000E+01 volume 0.75192E+01 ppm1 4 243 ppm2 1.108
ASSI { 9732}
(( segid "PROT" and resid 60 and name HB2 ))
(( segid "PROT" and resid 22 and name HD1%))
2.600 1.700 1.700 peak 9732 weight 0.10000E+01 volume 0.32675E+01 ppm1 4.068 ppm2 1.106
ASSI { 9742}
(( segid "PROT" and resid 110 and name HA ))
(( segid "PROT" and resid 110 and name HG11))
2.300 2.300 2.200 peak 9742 weight 0.10000E+01 volume 0.76467E+01 ppm1 3.864 ppm2 1.164
ASSI { 9752}
(( segid "PROT" and resid 22 and name HB1 ))
(( segid "PROT" and resid 22 and name HD1%))
2.300 1.300 1.300 peak 9752 weight 0.10000E+01 volume 0.68112E+01 ppm1 2.133 ppm2 1.110
ASSI { 9762}
(( segid "PROT" and resid 22 and name HG ))
(( segid "PROT" and resid 22 and name HD1%))
2.100 1.100 1.100 peak 9762 weight 0.10000E+01 volume 0.12147E+02 ppm1 1.796 ppm2 1.106
ASSI { 9832}
(( segid "PROT" and resid 78 and name HA ))
(( segid "PROT" and resid 78 and name HD1%))
2.500 1.600 1.600 peak 9832 weight 0.10000E+01 volume 0.38272E+01 ppm1 3.413 ppm2 0.094
ASSI { 9842}
(( segid "PROT" and resid 25 and name HG1%))
(( segid "PROT" and resid 78 and name HD1%))
2.400 1.400 1.400 peak 9842 weight 0.10000E+01 volume 0.54518E+01 ppm1 1.247 ppm2 0.094
ASSI { 9852}
(( segid "PROT" and resid 25 and name HG2%))
(( segid "PROT" and resid 78 and name HD1%))
2.300 1.300 1.300 peak 9852 weight 0.10000E+01 volume 0.77910E+01 ppm1 1.063 ppm2 0.094
ASSI { 9862}
(( segid "PROT" and resid 78 and name HG ))
(( segid "PROT" and resid 78 and name HD1%))
2.100 1.100 1.100 peak 9862 weight 0.10000E+01 volume 0.12211E+02 ppm1 0.695 ppm2 0.096
ASSI { 9872}
(( segid "PROT" and resid 78 and name HB1 ))
(( segid "PROT" and resid 78 and name HD1%))
2.300 1 300 1.300 peak 9872 weight 0.10000E+01 volume 0.76579E+01 ppm1 0.746 ppm2 0.098
ASSI { 9882}
(( segid "PROT" and resid 78 and name HD2%))
(( segid "PROT" and resid 78 and name HD1%))
1.900 0.900 0.900 peak 9882 weight 0.10000E+01 volume 0.23626E+02 ppm1 0.198 ppm2 0.092
ASSI { 9892}
(( segid "PROT" and resid 68 and name HD% ))

```

```

( segid "PROT" and resid 73 and name HD1%)
3.000 2.200 2.200 peak 9892 weight 0.10000E+01 volume 0.15029E+01 ppm1 7.197 ppm2 0.975
ASSI { 9922}
(( segid "PROT" and resid 68 and name HA ))
( segid "PROT" and resid 73 and name HD1%)
2.700 1.800 1.800 peak 9922 weight 0.10000E+01 volume 0.24042E+01 ppm1 4.579 ppm2 0.973
ASSI { 9932}
(( segid "PROT" and resid 11 and name HA ))
( segid "PROT" and resid 14 and name HD1%)
2.900 2.100 2.100 peak 9932 weight 0.10000E+01 volume 0.17985E+01 ppm1 4.374 ppm2 0.853
ASSI { 9942}
(( segid "PROT" and resid 73 and name HA ))
( segid "PROT" and resid 73 and name HD1%)
2.600 1.700 1.700 peak 9942 weight 0.10000E+01 volume 0.35846E+01 ppm1 4.253 ppm2 0.976
ASSI { 9962}
(( segid "PROT" and resid 14 and name HA ))
( segid "PROT" and resid 14 and name HD1%)
2.400 1.400 1.400 peak 9962 weight 0.10000E+01 volume 0.48248E+01 ppm1 4.104 ppm2 0.849
ASSI { 9972}
(( segid "PROT" and resid 70 and name HB2 ))
( segid "PROT" and resid 73 and name HD1%)
2.800 2.000 2.000 peak 9972 weight 0.10000E+01 volume 0.22200E+01 ppm1 3.786 ppm2 0.978
ASSI { 9992}
(( segid "PROT" and resid 73 and name HB1 ))
( segid "PROT" and resid 73 and name HD1%)
2.300 1.300 1.300 peak 9992 weight 0.10000E+01 volume 0.72852E+01 ppm1 2.029 ppm2 0.973
ASSI {10002}
(( segid "PROT" and resid 73 and name HB2 ))
( segid "PROT" and resid 73 and name HD1%)
2.300 1.300 1.300 peak 10002 weight 0.10000E+01 volume 0.72588E+01 ppm1 1.916 ppm2 0.972
ASSI {10052}
(( segid "PROT" and resid 14 and name HB2 ))
( segid "PROT" and resid 14 and name HD1%)
2.200 1.200 1.200 peak 10052 weight 0.10000E+01 volume 0.93159E+01 ppm1 1.590 ppm2 0.845
ASSI {10062}
(( segid "PROT" and resid 33 and name HD2 ))
(( segid "PROT" and resid 33 and name HG1 ))
2.900 2.100 2.100 peak 10062 weight 0.10000E+01 volume 0.15987E+01 ppm1 1.574 ppm2 0.274
ASSI {10072}
(( segid "PROT" and resid 33 and name HD2 ))
(( segid "PROT" and resid 33 and name HG2 ))
2.900 2.100 2.100 peak 10072 weight 0.10000E+01 volume 0.15869E+01 ppm1 1.572 ppm2 -0.867
ASSI {10132}
(( segid "PROT" and resid 33 and name HG2 ))
(( segid "PROT" and resid 33 and name HG1 ))
2.500 1.600 1.600 peak 10132 weight 0.10000E+01 volume 0.43453E+01 ppm1 -0.869 ppm2 0.275
ASSI {10182}
( segid "PROT" and resid 74 and name HD%)
( segid "PROT" and resid 18 and name HD1%)
2.800 2.000 2.000 peak 10182 weight 0.10000E+01 volume 0.23158E+01 ppm1 6.436 ppm2 0.515
ASSI {10192}
(( segid "PROT" and resid 63 and name HA ))
( segid "PROT" and resid 63 and name HD2%)
2.300 1.300 1.300 peak 10192 weight 0.10000E+01 volume 0.61524E+01 ppm1 4.722 ppm2 1.076
ASSI {10252}
(( segid "PROT" and resid 15 and name HA ))
( segid "PROT" and resid 18 and name HD1%)
2.500 1.600 1.600 peak 10252 weight 0.10000E+01 volume 0.38191E+01 ppm1 4.060 ppm2 0.514
ASSI {10262}
(( segid "PROT" and resid 110 and name HA ))
( segid "PROT" and resid 115 and name HD1%)
2.500 1.600 1.600 peak 10262 weight 0.10000E+01 volume 0.43512E+01 ppm1 3.859 ppm2 0.753
ASSI {10292}
(( segid "PROT" and resid 68 and name HB1 ))
( segid "PROT" and resid 18 and name HD1%)
2.600 1.700 1.700 peak 10292 weight 0.10000E+01 volume 0.32587E+01 ppm1 3.105 ppm2 0.509
ASSI {10302}
(( segid "PROT" and resid 66 and name HD2 ))
(( segid "PROT" and resid 66 and name HB2 ))
3.000 2.200 2.200 peak 10302 weight 0.10000E+01 volume 0.15198E+01 ppm1 3.068 ppm2 2.051
ASSI {10312}
(( segid "PROT" and resid 68 and name HB2 ))
( segid "PROT" and resid 18 and name HD1%)
2.400 1.400 1.400 peak 10312 weight 0.10000E+01 volume 0.47243E+01 ppm1 2.967 ppm2 0.515
ASSI {10322}
(( segid "PROT" and resid 74 and name HB2 ))
( segid "PROT" and resid 18 and name HD1%)
2.700 1.800 1.800 peak 10322 weight 0.10000E+01 volume 0.25991E+01 ppm1 2.427 ppm2 0.515
ASSI {10332}
(( segid "PROT" and resid 63 and name HB1 ))
( segid "PROT" and resid 63 and name HD2%)
2.600 1.700 1.700 peak 10332 weight 0.10000E+01 volume 0.35188E+01 ppm1 2.354 ppm2 1.078
ASSI {10342}
(( segid "PROT" and resid 66 and name HB1 ))
(( segid "PROT" and resid 66 and name HB2 ))
2.200 1.200 1.200 peak 10342 weight 0.10000E+01 volume 0.86683E+01 ppm1 2.141 ppm2 2.046
ASSI {10382}
(( segid "PROT" and resid 8 and name HB2 ))
( segid "PROT" and resid 115 and name HD1%)

```

2.600	1.700	1.700	peak 10382	weight	0.10000E+01	volume	0.34114E+01	ppm1	1.908	ppm2	0.758
ASSI {10392}											
((segid "PROT" and resid 14 and name HB1))											
(segid "PROT" and resid 18 and name HD1%)											
2.900	2.100	2.100	peak 10392	weight	0.10000E+01	volume	0.18010E+01	ppm1	1.884	ppm2	0.515
ASSI {10402}											
((segid "PROT" and resid 63 and name HG))											
(segid "PROT" and resid 63 and name HD2%)											
2.200	1.200	1.200	peak 10402	weight	0.10000E+01	volume	0.88532E+01	ppm1	1.852	ppm2	1.078
ASSI {10412}											
((segid "PROT" and resid 56 and name HG))											
(segid "PROT" and resid 102 and name HD1%)											
2.100	2.100	2.400	peak 10412	weight	0.10000E+01	volume	0.10879E+02	ppm1	1.766	ppm2	0.757
ASSI {10422}											
((segid "PROT" and resid 18 and name HG))											
(segid "PROT" and resid 18 and name HD1%)											
2.400	1.400	1.400	peak 10422	weight	0.10000E+01	volume	0.59544E+01	ppm1	1.702	ppm2	0.514
ASSI {10432}											
((segid "PROT" and resid 66 and name HG1))											
((segid "PROT" and resid 66 and name HB2))											
2.500	1.600	1.600	peak 10432	weight	0.10000E+01	volume	0.41346E+01	ppm1	1.600	ppm2	2.049
ASSI {10442}											
((segid "PROT" and resid 66 and name HG1))											
((segid "PROT" and resid 66 and name HB1))											
2.500	1.600	1.600	peak 10442	weight	0.10000E+01	volume	0.41383E+01	ppm1	1.601	ppm2	2.130
ASSI {10452}											
((segid "PROT" and resid 18 and name HB1))											
(segid "PROT" and resid 63 and name HD2%)											
2.500	1.600	1.600	peak 10452	weight	0.10000E+01	volume	0.43181E+01	ppm1	1.557	ppm2	1.078
ASSI {10462}											
((segid "PROT" and resid 18 and name HB1))											
(segid "PROT" and resid 18 and name HD1%)											
2.400	1.400	1.400	peak 10462	weight	0.10000E+01	volume	0.55398E+01	ppm1	1.554	ppm2	0.514
ASSI {10482}											
((segid "PROT" and resid 86 and name HG1))											
((segid "PROT" and resid 86 and name HG2))											
2.300	1.300	1.300	peak 10482	weight	0.10000E+01	volume	0.61301E+01	ppm1	1.341	ppm2	0.166
ASSI {10492}											
(segid "PROT" and resid 17 and name HG2%)											
(segid "PROT" and resid 115 and name HD1%)											
2.200	1.200	1.200	peak 10492	weight	0.10000E+01	volume	0.99350E+01	ppm1	1.178	ppm2	0.748
ASSI {10522}											
(segid "PROT" and resid 14 and name HD2%)											
(segid "PROT" and resid 18 and name HD1%)											
2.200	1.200	1.200	peak 10522	weight	0.10000E+01	volume	0.78947E+01	ppm1	0.826	ppm2	0.513
ASSI {10532}											
(segid "PROT" and resid 110 and name HD1%)											
(segid "PROT" and resid 115 and name HD1%)											
2.600	2.600	1.900	peak 10532	weight	0.10000E+01	volume	0.34067E+01	ppm1	0.568	ppm2	0.761
ASSI {10542}											
(segid "PROT" and resid 18 and name HD1%)											
(segid "PROT" and resid 63 and name HD2%)											
2.400	1.400	1.400	peak 10542	weight	0.10000E+01	volume	0.48392E+01	ppm1	0.516	ppm2	1.079
ASSI {10552}											
((segid "PROT" and resid 18 and name HB2))											
(segid "PROT" and resid 63 and name HD2%)											
2.700	1.800	1.800	peak 10552	weight	0.10000E+01	volume	0.25611E+01	ppm1	0.343	ppm2	1.079
ASSI {10562}											
((segid "PROT" and resid 18 and name HB2))											
(segid "PROT" and resid 18 and name HD1%)											
2.500	1.600	1.600	peak 10562	weight	0.10000E+01	volume	0.41021E+01	ppm1	0.346	ppm2	0.517
ASSI {10592}											
(segid "PROT" and resid 18 and name HD2%)											
(segid "PROT" and resid 115 and name HD1%)											
2.300	1.300	1.300	peak 10592	weight	0.10000E+01	volume	0.64278E+01	ppm1	-0.160	ppm2	0.749
ASSI {10632}											
(segid "PROT" and resid 82 and name HE%)											
(segid "PROT" and resid 102 and name HD1%)											
2.400	1.400	1.400	peak 10632	weight	0.10000E+01	volume	0.49504E+01	ppm1	6.476	ppm2	0.761
ASSI {10662}											
((segid "PROT" and resid 104 and name HA))											
(segid "PROT" and resid 104 and name HG1))											
2.300	1.300	1.300	peak 10662	weight	0.10000E+01	volume	0.62943E+01	ppm1	4.103	ppm2	1.550
ASSI {10672}											
((segid "PROT" and resid 104 and name HA))											
(segid "PROT" and resid 104 and name HG2))											
2.300	1.300	1.300	peak 10672	weight	0.10000E+01	volume	0.73311E+01	ppm1	4.097	ppm2	1.453
ASSI {10682}											
((segid "PROT" and resid 104 and name HE1))											
(segid "PROT" and resid 104 and name HG1))											
2.100	1.100	1.100	peak 10682	weight	0.10000E+01	volume	0.11157E+02	ppm1	3.028	ppm2	1.569
ASSI {10702}											
((segid "PROT" and resid 111 and name HE1))											
(segid "PROT" and resid 111 and name HG1))											
2.600	1.700	1.700	peak 10702	weight	0.10000E+01	volume	0.33124E+01	ppm1	2.934	ppm2	1.450
ASSI {10762}											
((segid "PROT" and resid 102 and name HB1))											
(segid "PROT" and resid 102 and name HD1%)											
2.300	1.300	1.300	peak 10762	weight	0.10000E+01	volume	0.66432E+01	ppm1	1.468	ppm2	0.764

```

ASSI {10772}
(( segid "PROT" and resid 102 and name HB2 ))
( segid "PROT" and resid 102 and name HD1%)
2.300 1.300 1.300 peak 10772 weight 0.10000E+01 volume 0.71507E+01 ppm1 1.261 ppm2 0.761
ASSI {10782}
( segid "PROT" and resid 25 and name HG2%)
( segid "PROT" and resid 102 and name HD1%)
2.100 1.100 1.100 peak 10782 weight 0.10000E+01 volume 0.10874E+02 ppm1 1.072 ppm2 0.760
ASSI {10792}
( segid "PROT" and resid 116 and name HG2%)
(( segid "PROT" and resid 111 and name HG1 ))
2.700 1.800 1.800 peak 10792 weight 0.10000E+01 volume 0.28695E+01 ppm1 0.835 ppm2 1.453
ASSI {10802}
(( segid "PROT" and resid 64 and name HA ))
(( segid "PROT" and resid 64 and name HG1 ))
2.500 1.600 1.600 peak 10802 weight 0.10000E+01 volume 0.42177E+01 ppm1 4.377 ppm2 1.650
ASSI {10862}
(( segid "PROT" and resid 16 and name HB2 ))
(( segid "PROT" and resid 19 and name HG1 ))
2.900 2.100 2.100 peak 10862 weight 0.10000E+01 volume 0.17444E+01 ppm1 3.940 ppm2 1.316
ASSI {10902}
( segid "PROT" and resid 14 and name HD2%)
(( segid "PROT" and resid 18 and name HG ))
2.700 1.800 1.800 peak 10902 weight 0.10000E+01 volume 0.24419E+01 ppm1 0.833 ppm2 1.690
ASSI {10932}
(( segid "PROT" and resid 81 and name HB ))
( segid "PROT" and resid 78 and name HD2%)
2.600 1.700 1.700 peak 10932 weight 0.10000E+01 volume 0.30227E+01 ppm1 1.467 ppm2 0.196
ASSI {10942}
( segid "PROT" and resid 59 and name HE%)
( segid "PROT" and resid 78 and name HD2%)
2.400 1.400 1.400 peak 10942 weight 0.10000E+01 volume 0.59847E+01 ppm1 1.310 ppm2 0.194
ASSI {10952}
(( segid "PROT" and resid 50 and name HB ))
(( segid "PROT" and resid 50 and name HG12))
2.400 1.400 1.400 peak 10952 weight 0.10000E+01 volume 0.59613E+01 ppm1 1.249 ppm2 0.193
ASSI {10992}
(( segid "PROT" and resid 50 and name HG12))
(( segid "PROT" and resid 50 and name HG11))
2.500 1.600 1.600 peak 10992 weight 0.10000E+01 volume 0.39414E+01 ppm1 0.185 ppm2 0.827
ASSI {11052}
(( segid "PROT" and resid 25 and name HA ))
( segid "PROT" and resid 102 and name HD2%)
2.500 1.600 1.600 peak 11052 weight 0.10000E+01 volume 0.41975E+01 ppm1 3.869 ppm2 0.766
ASSI {11072}
(( segid "PROT" and resid 78 and name HA ))
( segid "PROT" and resid 78 and name HD2%)
2.200 1.200 1.200 peak 11072 weight 0.10000E+01 volume 0.82572E+01 ppm1 3.416 ppm2 0.198
ASSI {11082}
(( segid "PROT" and resid 105 and name HB2 ))
( segid "PROT" and resid 102 and name HD2%)
2.500 1.600 1.600 peak 11082 weight 0.10000E+01 volume 0.41341E+01 ppm1 3.101 ppm2 0.766
ASSI {11092}
(( segid "PROT" and resid 28 and name HB1 ))
( segid "PROT" and resid 102 and name HD2%)
2.400 1.400 1.400 peak 11092 weight 0.10000E+01 volume 0.49393E+01 ppm1 3.023 ppm2 0.767
ASSI {11102}
(( segid "PROT" and resid 28 and name HB2 ))
( segid "PROT" and resid 102 and name HD2%)
2.600 1.700 1.700 peak 11102 weight 0.10000E+01 volume 0.32553E+01 ppm1 2.819 ppm2 0.763
ASSI {11112}
(( segid "PROT" and resid 102 and name HB2 ))
( segid "PROT" and resid 102 and name HD2%)
2.200 1.200 1.200 peak 11112 weight 0.10000E+01 volume 0.80020E+01 ppm1 1.257 ppm2 0.766
ASSI {11132}
( segid "PROT" and resid 25 and name HG2%)
( segid "PROT" and resid 78 and name HD2%)
2.200 1.200 1.200 peak 11132 weight 0.10000E+01 volume 0.84055E+01 ppm1 1.062 ppm2 0.196
ASSI {11142}
(( segid "PROT" and resid 78 and name HG ))
( segid "PROT" and resid 78 and name HD2%)
2.000 1.000 1.000 peak 11142 weight 0.10000E+01 volume 0.17074E+02 ppm1 0.691 ppm2 0.194
ASSI {11152}
(( segid "PROT" and resid 78 and name HB2 ))
( segid "PROT" and resid 78 and name HD2%)
2.300 1.300 1.300 peak 11152 weight 0.10000E+01 volume 0.74312E+01 ppm1 0.500 ppm2 0.195
ASSI {11182}
(( segid "PROT" and resid 22 and name HA ))
( segid "PROT" and resid 22 and name HD2%)
2.100 1.100 1.100 peak 11182 weight 0.10000E+01 volume 0.11230E+02 ppm1 4.153 ppm2 1.051
ASSI {11192}
(( segid "PROT" and resid 56 and name HA ))
( segid "PROT" and resid 22 and name HD2%)
2.600 1.700 1.700 peak 11192 weight 0.10000E+01 volume 0.30625E+01 ppm1 4.068 ppm2 1.051
ASSI {11202}
(( segid "PROT" and resid 25 and name HB ))
( segid "PROT" and resid 22 and name HD2%)
2.700 1.800 1.800 peak 11202 weight 0.10000E+01 volume 0.24545E+01 ppm1 2.446 ppm2 1.047
ASSI {11212}

```


1.0000E+01 volume 0.56798E+01 ppm1 2.136 ppm2 1.050
 1.0000E+01 volume 0.41435E+01 ppm1 1.915 ppm2 1.051
 1.0000E+01 volume 0.99228E+01 ppm1 1.793 ppm2 1.049
 1.0000E+01 volume 0.61801E+01 ppm1 1.309 ppm2 1.049
 1.0000E+01 volume 0.28974E+01 ppm1 0.196 ppm2 1.049
 1.0000E+01 volume 0.18093E+01 ppm1 0.095 ppm2 1.049
 1.0000E+01 volume 0.13997E+02 ppm1 4.260 ppm2 0.928
 1.0000E+01 volume 0.52914E+01 ppm1 2.029 ppm2 0.928
 1.0000E+01 volume 0.73295E+01 ppm1 1.916 ppm2 0.924
 1.0000E+01 volume 0.73274E+01 ppm1 1.178 ppm2 0.784
 1.0000E+01 volume 0.13990E+02 ppm1 4.258 ppm2 0.783
 1.0000E+01 volume 0.17448E+02 ppm1 4.086 ppm2 0.830
 1.0000E+01 volume 0.10938E+02 ppm1 1.899 ppm2 0.824
 1.0000E+01 volume 0.93323E+01 ppm1 1.426 ppm2 0.838
 1.0000E+01 volume 0.99743E+01 ppm1 -0.160 ppm2 0.822
 1.0000E+01 volume 0.32864E+01 ppm1 6.951 ppm2 1.244
 1.0000E+01 volume 0.33649E+01 ppm1 4.154 ppm2 1.248
 1.0000E+01 volume 0.30836E+01 ppm1 4.000 ppm2 1.243
 1.0000E+01 volume 0.89668E+01 ppm1 3.867 ppm2 1.246
 1.0000E+01 volume 0.20827E+01 ppm1 3.136 ppm2 1.245
 1.0000E+01 volume 0.10379E+02 ppm1 2.445 ppm2 1.245
 1.0000E+01 volume 0.15965E+01 ppm1 1.595 ppm2 1.239

```

(( segid "PROT" and resid 22 and name HB1 ))
( segid "PROT" and resid 22 and name HD2%)
2.400 1.400 1.400 peak 11212 weight 0.10000E+01 volume 0.56798E+01 ppm1 2.136 ppm2 1.050
ASSI {11222}
(( segid "PROT" and resid 59 and name HB2 ))
( segid "PROT" and resid 22 and name HD2%)
2.500 1.600 1.600 peak 11222 weight 0.10000E+01 volume 0.41435E+01 ppm1 1.915 ppm2 1.051
ASSI {11232}
(( segid "PROT" and resid 22 and name HG ))
( segid "PROT" and resid 22 and name HD2%)
2.200 1.200 1.200 peak 11232 weight 0.10000E+01 volume 0.99228E+01 ppm1 1.793 ppm2 1.049
ASSI {11242}
( segid "PROT" and resid 59 and name HE%)
( segid "PROT" and resid 22 and name HD2%)
2.300 1.300 1.300 peak 11242 weight 0.10000E+01 volume 0.61801E+01 ppm1 1.309 ppm2 1.049
ASSI {11272}
( segid "PROT" and resid 78 and name HD2%)
( segid "PROT" and resid 22 and name HD2%)
2.700 1.800 1.800 peak 11272 weight 0.10000E+01 volume 0.28974E+01 ppm1 0.196 ppm2 1.049
ASSI {11282}
( segid "PROT" and resid 78 and name HD1%)
( segid "PROT" and resid 22 and name HD2%)
2.900 2.100 2.100 peak 11282 weight 0.10000E+01 volume 0.18093E+01 ppm1 0.095 ppm2 1.049
ASSI {11302}
(( segid "PROT" and resid 73 and name HA ))
( segid "PROT" and resid 73 and name HD2%)
2.000 1.000 1.000 peak 11302 weight 0.10000E+01 volume 0.13997E+02 ppm1 4.260 ppm2 0.928
ASSI {11312}
(( segid "PROT" and resid 73 and name HB1 ))
( segid "PROT" and resid 73 and name HD2%)
2.400 1.400 1.400 peak 11312 weight 0.10000E+01 volume 0.52914E+01 ppm1 2.029 ppm2 0.928
ASSI {11322}
(( segid "PROT" and resid 73 and name HB2 ))
( segid "PROT" and resid 73 and name HD2%)
2.300 1.300 1.300 peak 11322 weight 0.10000E+01 volume 0.73295E+01 ppm1 1.916 ppm2 0.924
ASSI {11342}
( segid "PROT" and resid 17 and name HG2%)
( segid "PROT" and resid 115 and name HD2%)
2.300 1.300 1.300 peak 11342 weight 0.10000E+01 volume 0.73274E+01 ppm1 1.178 ppm2 0.784
ASSI {11352}
(( segid "PROT" and resid 115 and name HA ))
( segid "PROT" and resid 115 and name HD2%)
2.000 1.000 1.000 peak 11352 weight 0.10000E+01 volume 0.13990E+02 ppm1 4.258 ppm2 0.783
ASSI {11362}
(( segid "PROT" and resid 14 and name HA ))
( segid "PROT" and resid 14 and name HD2%)
2.000 1.000 1.000 peak 11362 weight 0.10000E+01 volume 0.17448E+02 ppm1 4.086 ppm2 0.830
ASSI {11382}
(( segid "PROT" and resid 14 and name HB1 ))
( segid "PROT" and resid 14 and name HD2%)
2.100 1.100 1.100 peak 11382 weight 0.10000E+01 volume 0.10938E+02 ppm1 1.899 ppm2 0.824
ASSI {11412}
(( segid "PROT" and resid 14 and name HG ))
( segid "PROT" and resid 14 and name HD2%)
2.200 1.200 1.200 peak 11412 weight 0.10000E+01 volume 0.93323E+01 ppm1 1.426 ppm2 0.838
ASSI {11432}
( segid "PROT" and resid 18 and name HD2%)
( segid "PROT" and resid 14 and name HD2%)
2.200 1.200 1.200 peak 11432 weight 0.10000E+01 volume 0.99743E+01 ppm1 -0.160 ppm2 0.822
ASSI {11462}
( segid "PROT" and resid 106 and name HD%)
( segid "PROT" and resid 25 and name HG1%)
2.600 1.700 1.700 peak 11462 weight 0.10000E+01 volume 0.32864E+01 ppm1 6.951 ppm2 1.244
ASSI {11472}
(( segid "PROT" and resid 22 and name HA ))
( segid "PROT" and resid 25 and name HG1%)
2.600 1.700 1.700 peak 11472 weight 0.10000E+01 volume 0.33649E+01 ppm1 4.154 ppm2 1.248
ASSI {11482}
(( segid "PROT" and resid 106 and name HA ))
( segid "PROT" and resid 25 and name HG1%)
2.600 1.700 1.700 peak 11482 weight 0.10000E+01 volume 0.30836E+01 ppm1 4.000 ppm2 1.243
ASSI {11492}
(( segid "PROT" and resid 25 and name HA ))
( segid "PROT" and resid 25 and name HG1%)
2.200 1.200 1.200 peak 11492 weight 0.10000E+01 volume 0.89668E+01 ppm1 3.867 ppm2 1.246
ASSI {11502}
(( segid "PROT" and resid 106 and name HB2 ))
( segid "PROT" and resid 25 and name HG1%)
2.800 2.000 2.000 peak 11502 weight 0.10000E+01 volume 0.20827E+01 ppm1 3.136 ppm2 1.245
ASSI {11532}
(( segid "PROT" and resid 25 and name HB ))
( segid "PROT" and resid 25 and name HG1%)
2.100 1.100 1.100 peak 11532 weight 0.10000E+01 volume 0.10379E+02 ppm1 2.445 ppm2 1.245
ASSI {11552}
(( segid "PROT" and resid 102 and name HG ))
( segid "PROT" and resid 25 and name HG1%)
2.900 2.100 2.100 peak 11552 weight 0.10000E+01 volume 0.15965E+01 ppm1 1.595 ppm2 1.239
ASSI {11562}
( segid "PROT" and resid 25 and name HG2%)

```

```

( segid "PROT" and resid 25 and name HG1%)
1.900 0.900 0.900 peak 11562 weight 0.10000E+01 volume 0.22735E+02 ppm1 1.069 ppm2 1.243
ASSI {11572}
( segid "PROT" and resid 102 and name HD2%)
( segid "PROT" and resid 25 and name HG1%)
2.400 1.400 1.400 peak 11572 weight 0.10000E+01 volume 0.56418E+01 ppm1 0.764 ppm2 1.242
ASSI {11592}
( segid "PROT" and resid 78 and name HD2%)
( segid "PROT" and resid 25 and name HG1%)
2.600 1.700 1.700 peak 11592 weight 0.10000E+01 volume 0.31395E+01 ppm1 0.196 ppm2 1.242
ASSI {11612}
(( segid "PROT" and resid 41 and name HB ))
( segid "PROT" and resid 41 and name HG2%)
1.900 0.900 0.900 peak 11612 weight 0.10000E+01 volume 0.22674E+02 ppm1 4.345 ppm2 1.320
ASSI {11632}
(( segid "PROT" and resid 39 and name HB2 ))
( segid "PROT" and resid 41 and name HG2%)
2.800 2.000 2.000 peak 11632 weight 0.10000E+01 volume 0.20175E+01 ppm1 1.958 ppm2 1.319
ASSI {11642}
(( segid "PROT" and resid 59 and name HB2 ))
( segid "PROT" and resid 56 and name HD2%)
2.700 1.800 1.800 peak 11642 weight 0.10000E+01 volume 0.27107E+01 ppm1 1.922 ppm2 0.680
ASSI {11662}
(( segid "PROT" and resid 56 and name HG ))
( segid "PROT" and resid 56 and name HD2%)
2.200 1.200 1.200 peak 11662 weight 0.10000E+01 volume 0.99064E+01 ppm1 1.764 ppm2 0.678
ASSI {11672}
(( segid "PROT" and resid 39 and name HD2 ))
( segid "PROT" and resid 41 and name HG2%)
2.900 2.100 2.100 peak 11672 weight 0.10000E+01 volume 0.17126E+01 ppm1 1.680 ppm2 1.313
ASSI {11682}
(( segid "PROT" and resid 56 and name HB2 ))
( segid "PROT" and resid 56 and name HD2%)
2.500 1.600 1.600 peak 11682 weight 0.10000E+01 volume 0.46505E+01 ppm1 1.451 ppm2 0.678
ASSI {11692}
( segid "PROT" and resid 78 and name HD2%)
( segid "PROT" and resid 56 and name HD2%)
2.300 1.300 1.300 peak 11692 weight 0.10000E+01 volume 0.78069E+01 ppm1 0.194 ppm2 0.677
ASSI {11702}
( segid "PROT" and resid 78 and name HD1%)
( segid "PROT" and resid 56 and name HD2%)
2.500 1.600 1.600 peak 11702 weight 0.10000E+01 volume 0.38946E+01 ppm1 0.097 ppm2 0.678
ASSI {11722}
(( segid "PROT" and resid 54 and name HA ))
( segid "PROT" and resid 81 and name HG1%)
2.800 2.000 2.000 peak 11722 weight 0.10000E+01 volume 0.19593E+01 ppm1 4.986 ppm2 0.503
ASSI {11732}
(( segid "PROT" and resid 55 and name HA ))
( segid "PROT" and resid 81 and name HG1%)
2.500 1.600 1.600 peak 11732 weight 0.10000E+01 volume 0.38747E+01 ppm1 4.778 ppm2 0.507
ASSI {11742}
(( segid "PROT" and resid 83 and name HB ))
( segid "PROT" and resid 83 and name HG2%)
1.900 0.900 0.900 peak 11742 weight 0.10000E+01 volume 0.21486E+02 ppm1 4.240 ppm2 1.343
ASSI {11752}
(( segid "PROT" and resid 83 and name HA ))
( segid "PROT" and resid 83 and name HG2%)
2.000 1.000 1.000 peak 11752 weight 0.10000E+01 volume 0.15158E+02 ppm1 3.894 ppm2 1.343
ASSI {11772}
(( segid "PROT" and resid 78 and name HA ))
( segid "PROT" and resid 81 and name HG1%)
2.300 1.300 1.300 peak 11772 weight 0.10000E+01 volume 0.69671E+01 ppm1 3.419 ppm2 0.509
ASSI {11782}
(( segid "PROT" and resid 81 and name HA ))
( segid "PROT" and resid 81 and name HG1%)
2.100 1.100 1.100 peak 11782 weight 0.10000E+01 volume 0.10502E+02 ppm1 3.127 ppm2 0.508
ASSI {11792}
(( segid "PROT" and resid 54 and name HG1 ))
( segid "PROT" and resid 81 and name HG1%)
2.500 1.600 1.600 peak 11792 weight 0.10000E+01 volume 0.42195E+01 ppm1 2.741 ppm2 0.511
ASSI {11812}
(( segid "PROT" and resid 25 and name HB ))
( segid "PROT" and resid 25 and name HG2%)
2.100 1.100 1.100 peak 11812 weight 0.10000E+01 volume 0.10819E+02 ppm1 2.445 ppm2 1.073
ASSI {11832}
(( segid "PROT" and resid 53 and name HG2 ))
( segid "PROT" and resid 38 and name HG1%)
2.000 2.000 2.500 peak 11832 weight 0.10000E+01 volume 0.15230E+02 ppm1 1.938 ppm2 0.498
ASSI {11852}
(( segid "PROT" and resid 81 and name HB ))
( segid "PROT" and resid 81 and name HG1%)
2.100 1.100 1.100 peak 11852 weight 0.10000E+01 volume 0.10363E+02 ppm1 1.466 ppm2 0.509
ASSI {11862}
(( segid "PROT" and resid 38 and name HB ))
( segid "PROT" and resid 38 and name HG1%)
2.100 1.100 1.100 peak 11862 weight 0.10000E+01 volume 0.12690E+02 ppm1 1.072 ppm2 0.496
ASSI {11872}
( segid "PROT" and resid 43 and name HB%)
( segid "PROT" and resid 38 and name HG1%)

```

2.600	1.700	1.700	peak 11872	weight	0.10000E+01	volume	0.32089E+01	ppm1	0.992	ppm2	0.499
ASSI {11882}											
{ segid "PROT" and resid 56 and name HD2% }											
{ segid "PROT" and resid 25 and name HG2% }											
2.300	1.300	1.300	peak 11882	weight	0.10000E+01	volume	0.66325E+01	ppm1	0.678	ppm2	1.074
ASSI {11892}											
{ segid "PROT" and resid 56 and name HD2% }											
{ segid "PROT" and resid 81 and name HG1% }											
2.300	1.300	1.300	peak 11892	weight	0.10000E+01	volume	0.73060E+01	ppm1	0.678	ppm2	0.508
ASSI {11912}											
{ segid "PROT" and resid 81 and name HG2% }											
{ segid "PROT" and resid 81 and name HG1% }											
2.000	1.000	1.000	peak 11912	weight	0.10000E+01	volume	0.18518E+02	ppm1	0.157	ppm2	0.510
ASSI {11932}											
{ segid "PROT" and resid 38 and name HG2% }											
{ segid "PROT" and resid 38 and name HG1% }											
2.000	1.000	1.000	peak 11932	weight	0.10000E+01	volume	0.17706E+02	ppm1	-0.011	ppm2	0.496
ASSI {11942}											
{ segid "PROT" and resid 82 and name HD% }											
{ segid "PROT" and resid 81 and name HG2% }											
2.800	2.000	2.000	peak 11942	weight	0.10000E+01	volume	0.19816E+01	ppm1	6.692	ppm2	0.156
ASSI {11952}											
{ segid "PROT" and resid 82 and name HE% }											
{ segid "PROT" and resid 81 and name HG2% }											
2.900	2.100	2.100	peak 11952	weight	0.10000E+01	volume	0.16984E+01	ppm1	6.489	ppm2	0.157
ASSI {11962}											
{ segid "PROT" and resid 54 and name HA }											
{ segid "PROT" and resid 58 and name HG2% }											
2.900	2.100	2.100	peak 11962	weight	0.10000E+01	volume	0.16768E+01	ppm1	4.987	ppm2	1.099
ASSI {11972}											
{ segid "PROT" and resid 55 and name HA }											
{ segid "PROT" and resid 81 and name HG2% }											
2.800	2.000	2.000	peak 11972	weight	0.10000E+01	volume	0.22875E+01	ppm1	4.780	ppm2	0.156
ASSI {11982}											
{ segid "PROT" and resid 58 and name HB }											
{ segid "PROT" and resid 58 and name HG2% }											
1.900	0.900	0.900	peak 11982	weight	0.10000E+01	volume	0.18798E+02	ppm1	4.121	ppm2	1.097
ASSI {12002}											
{ segid "PROT" and resid 34 and name HD% }											
{ segid "PROT" and resid 81 and name HG2% }											
2.500	1.600	1.600	peak 12002	weight	0.10000E+01	volume	0.41738E+01	ppm1	7.185	ppm2	0.155
ASSI {12012}											
{ segid "PROT" and resid 34 and name HB1 }											
{ segid "PROT" and resid 81 and name HG2% }											
2.500	1.600	1.600	peak 12012	weight	0.10000E+01	volume	0.44360E+01	ppm1	3.515	ppm2	0.155
ASSI {12022}											
{ segid "PROT" and resid 85 and name HB1 }											
{ segid "PROT" and resid 81 and name HG2% }											
2.800	2.000	2.000	peak 12022	weight	0.10000E+01	volume	0.20402E+01	ppm1	3.415	ppm2	0.152
ASSI {12032}											
{ segid "PROT" and resid 81 and name HA }											
{ segid "PROT" and resid 81 and name HG2% }											
2.200	1.200	1.200	peak 12032	weight	0.10000E+01	volume	0.80317E+01	ppm1	3.128	ppm2	0.155
ASSI {12042}											
{ segid "PROT" and resid 34 and name HB2 }											
{ segid "PROT" and resid 81 and name HG2% }											
2.700	1.800	1.800	peak 12042	weight	0.10000E+01	volume	0.28427E+01	ppm1	2.638	ppm2	0.156
ASSI {12052}											
{ segid "PROT" and resid 57 and name HE1 }											
{ segid "PROT" and resid 58 and name HG2% }											
2.600	1.700	1.700	peak 12052	weight	0.10000E+01	volume	0.34800E+01	ppm1	2.612	ppm2	1.098
ASSI {12072}											
{ segid "PROT" and resid 81 and name HB }											
{ segid "PROT" and resid 81 and name HG2% }											
2.100	1.100	1.100	peak 12072	weight	0.10000E+01	volume	0.10373E+02	ppm1	1.469	ppm2	0.156
ASSI {12082}											
{ segid "PROT" and resid 102 and name HD1% }											
{ segid "PROT" and resid 81 and name HG2% }											
2.900	2.100	2.100	peak 12082	weight	0.10000E+01	volume	0.15611E+01	ppm1	0.755	ppm2	0.156
ASSI {12092}											
{ segid "PROT" and resid 56 and name HD2% }											
{ segid "PROT" and resid 81 and name HG2% }											
2.700	1.800	1.800	peak 12092	weight	0.10000E+01	volume	0.28031E+01	ppm1	0.680	ppm2	0.154
ASSI {12122}											
{ segid "PROT" and resid 69 and name HA }											
{ segid "PROT" and resid 69 and name HG1% }											
2.000	1.000	1.000	peak 12122	weight	0.10000E+01	volume	0.17855E+02	ppm1	4.119	ppm2	0.988
ASSI {12132}											
{ segid "PROT" and resid 38 and name HA }											
{ segid "PROT" and resid 38 and name HG2% }											
2.300	1.300	1.300	peak 12132	weight	0.10000E+01	volume	0.66566E+01	ppm1	3.494	ppm2	-0.010
ASSI {12142}											
{ segid "PROT" and resid 69 and name HB }											
{ segid "PROT" and resid 69 and name HG1% }											
2.000	1.000	1.000	peak 12142	weight	0.10000E+01	volume	0.18250E+02	ppm1	2.352	ppm2	0.990
ASSI {12172}											
{ segid "PROT" and resid 113 and name HB% }											
{ segid "PROT" and resid 17 and name HG2% }											
2.100	1.100	1.100	peak 12172	weight	0.10000E+01	volume	0.10423E+02	ppm1	1.411	ppm2	1.175

```

ASSI {12182}
  (( segid "PROT" and resid 38 and name HB ))
  ( segid "PROT" and resid 38 and name HG2% )
  2.200 1.200 1.200 peak 12182 weight 0.10000E+01 volume 0.92232E+01 ppm1 1.072 ppm2 -0.010
ASSI {12192}
  ( segid "PROT" and resid 43 and name HB% )
  ( segid "PROT" and resid 38 and name HG2% )
  2.100 1.100 1.100 peak 12192 weight 0.10000E+01 volume 0.10645E+02 ppm1 0.988 ppm2 -0.010
ASSI {12202}
  ( segid "PROT" and resid 21 and name HD1% )
  ( segid "PROT" and resid 17 and name HG2% )
  2.100 1.100 1.100 peak 12202 weight 0.10000E+01 volume 0.11281E+02 ppm1 0.654 ppm2 1.179
ASSI {12222}
  ( segid "PROT" and resid 18 and name HD2% )
  ( segid "PROT" and resid 17 and name HG2% )
  2.500 1.600 1.600 peak 12222 weight 0.10000E+01 volume 0.45180E+01 ppm1 -0.160 ppm2 1.179
ASSI {12232}
  (( segid "PROT" and resid 88 and name HA ))
  ( segid "PROT" and resid 49 and name HG2% )
  2.800 2.000 2.000 peak 12232 weight 0.10000E+01 volume 0.19275E+01 ppm1 4.335 ppm2 0.917
ASSI {12252}
  (( segid "PROT" and resid 49 and name HB ))
  ( segid "PROT" and resid 49 and name HG2% )
  2.100 1.100 1.100 peak 12252 weight 0.10000E+01 volume 0.11893E+02 ppm1 1.928 ppm2 0.910
ASSI {12262}
  ( segid "PROT" and resid 50 and name HD1% )
  ( segid "PROT" and resid 49 and name HG2% )
  2.300 1.300 1.300 peak 12262 weight 0.10000E+01 volume 0.67910E+01 ppm1 0.581 ppm2 0.912
ASSI {12302}
  (( segid "PROT" and resid 43 and name HA ))
  ( segid "PROT" and resid 43 and name HB% )
  2.200 1.200 1.200 peak 12302 weight 0.10000E+01 volume 0.99216E+01 ppm1 4.988 ppm2 0.987
ASSI {12312}
  (( segid "PROT" and resid 44 and name HD1 ))
  ( segid "PROT" and resid 43 and name HB% )
  2.900 2.100 2.100 peak 12312 weight 0.10000E+01 volume 0.17587E+01 ppm1 3.830 ppm2 0.988
ASSI {12322}
  (( segid "PROT" and resid 46 and name HB1 ))
  ( segid "PROT" and resid 43 and name HB% )
  2.500 1.600 1.600 peak 12322 weight 0.10000E+01 volume 0.47081E+01 ppm1 2.762 ppm2 0.987
ASSI {12332}
  (( segid "PROT" and resid 46 and name HB2 ))
  ( segid "PROT" and resid 43 and name HB% )
  2.500 1.600 1.600 peak 12332 weight 0.10000E+01 volume 0.40150E+01 ppm1 2.426 ppm2 0.984
ASSI {12342}
  (( segid "PROT" and resid 39 and name HG2 ))
  ( segid "PROT" and resid 43 and name HB% )
  2.800 2.000 2.000 peak 12342 weight 0.10000E+01 volume 0.20520E+01 ppm1 1.443 ppm2 0.986
ASSI {12352}
  ( segid "PROT" and resid 41 and name HG2% )
  ( segid "PROT" and resid 43 and name HB% )
  2.600 1.700 1.700 peak 12352 weight 0.10000E+01 volume 0.31831E+01 ppm1 1.342 ppm2 0.985
ASSI {12382}
  ( segid "PROT" and resid 34 and name HD% )
  ( segid "PROT" and resid 31 and name HB% )
  2.800 2.000 2.000 peak 12382 weight 0.10000E+01 volume 0.21740E+01 ppm1 7.180 ppm2 1.761
ASSI {12402}
  ( segid "PROT" and resid 74 and name HD% )
  ( segid "PROT" and resid 18 and name HD2% )
  2.700 1.800 1.800 peak 12402 weight 0.10000E+01 volume 0.27909E+01 ppm1 6.432 ppm2 -0.161
ASSI {12412}
  (( segid "PROT" and resid 31 and name HA ))
  ( segid "PROT" and resid 31 and name HB% )
  2.100 1.100 1.100 peak 12412 weight 0.10000E+01 volume 0.11588E+02 ppm1 4 438 ppm2 1.763
ASSI {12422}
  (( segid "PROT" and resid 14 and name HA ))
  ( segid "PROT" and resid 18 and name HD2% )
  2.500 1.600 1.600 peak 12422 weight 0.10000E+01 volume 0.46610E+01 ppm1 4.061 ppm2 -0.160
ASSI {12432}
  (( segid "PROT" and resid 26 and name HA ))
  ( segid "PROT" and resid 31 and name HB% )
  2.300 1.300 1.300 peak 12432 weight 0.10000E+01 volume 0.63967E+01 ppm1 3.932 ppm2 1.762
ASSI {12442}
  (( segid "PROT" and resid 18 and name HA ))
  ( segid "PROT" and resid 18 and name HD2% )
  2.100 1.100 1.100 peak 12442 weight 0.10000E+01 volume 0.11266E+02 ppm1 3.315 ppm2 -0.161
ASSI {12452}
  (( segid "PROT" and resid 28 and name HB1 ))
  ( segid "PROT" and resid 31 and name HB% )
  2.800 2.000 2.000 peak 12452 weight 0.10000E+01 volume 0.21964E+01 ppm1 3.014 ppm2 1.761
ASSI {12462}
  (( segid "PROT" and resid 74 and name HB1 ))
  ( segid "PROT" and resid 18 and name HD2% )
  2.700 1.800 1.800 peak 12462 weight 0.10000E+01 volume 0.27167E+01 ppm1 2.985 ppm2 -0.159
ASSI {12472}
  (( segid "PROT" and resid 35 and name HG1 ))
  ( segid "PROT" and resid 31 and name HB% )
  2.900 2.100 2.100 peak 12472 weight 0.10000E+01 volume 0.18022E+01 ppm1 2.893 ppm2 1.761
ASSI {12482}

```

```

(( segid "PROT" and resid 28 and name HB2 ))
( segid "PROT" and resid 31 and name HB% )
2.800 2.000 2.000 peak 12482 weight 0.10000E+01 volume 0.19169E+01 ppm1 2.827 ppm2 1.761
ASSI {12492}
(( segid "PROT" and resid 74 and name HB2 ))
( segid "PROT" and resid 18 and name HD2% )
2.900 2.100 2.100 peak 12492 weight 0.10000E+01 volume 0.16460E+01 ppm1 2.426 ppm2 -0.159
ASSI {12502}
( segid "PROT" and resid 35 and name HB% )
( segid "PROT" and resid 31 and name HB% )
2.500 1.600 1.600 peak 12502 weight 0.10000E+01 volume 0.46210E+01 ppm1 2.220 ppm2 1.761
ASSI {12512}
(( segid "PROT" and resid 14 and name HB1 ))
( segid "PROT" and resid 18 and name HD2% )
2.700 1.800 1.800 peak 12512 weight 0.10000E+01 volume 0.24259E+01 ppm1 1.907 ppm2 -0.160
ASSI {12522}
(( segid "PROT" and resid 18 and name HG ))
( segid "PROT" and resid 18 and name HD2% )
2.200 1.200 1.200 peak 12522 weight 0.10000E+01 volume 0.90471E+01 ppm1 1.706 ppm2 -0.160
ASSI {12532}
(( segid "PROT" and resid 18 and name HB1 ))
( segid "PROT" and resid 18 and name HD2% )
2.400 1.400 1.400 peak 12532 weight 0.10000E+01 volume 0.47694E+01 ppm1 1.563 ppm2 -0.162
ASSI {12552}
( segid "PROT" and resid 63 and name HD2% )
( segid "PROT" and resid 18 and name HD2% )
2.900 2.100 2.100 peak 12552 weight 0.10000E+01 volume 0.18027E+01 ppm1 1.078 ppm2 -0.159
ASSI {12572}
( segid "PROT" and resid 56 and name HD1% )
( segid "PROT" and resid 31 and name HB% )
2.300 1.300 1.300 peak 12572 weight 0.10000E+01 volume 0.76065E+01 ppm1 0.978 ppm2 1.761
ASSI {12592}
( segid "PROT" and resid 102 and name HD1% )
( segid "PROT" and resid 31 and name HB% )
2.100 1.100 1.100 peak 12592 weight 0.10000E+01 volume 0.13169E+02 ppm1 0.763 ppm2 1.762
ASSI {12612}
( segid "PROT" and resid 21 and name HD1% )
( segid "PROT" and resid 18 and name HD2% )
2.500 1.600 1.600 peak 12612 weight 0.10000E+01 volume 0.39733E+01 ppm1 0.654 ppm2 -0.158
ASSI {12622}
( segid "PROT" and resid 18 and name HD1% )
( segid "PROT" and resid 18 and name HD2% )
2.000 1.000 1.000 peak 12622 weight 0.10000E+01 volume 0.15661E+02 ppm1 0.515 ppm2 -0.160
ASSI {12632}
(( segid "PROT" and resid 18 and name HB2 ))
( segid "PROT" and resid 18 and name HD2% )
2.600 1.700 1.700 peak 12632 weight 0.10000E+01 volume 0.35201E+01 ppm1 0.341 ppm2 -0.159
ASSI {12642}
(( segid "PROT" and resid 113 and name HA ))
( segid "PROT" and resid 113 and name HB% )
1.900 0.900 0.900 peak 12642 weight 0.10000E+01 volume 0.23011E+02 ppm1 4.338 ppm2 1.411
ASSI {12672}
(( segid "PROT" and resid 115 and name HG ))
( segid "PROT" and resid 113 and name HB% )
2.300 1.300 1.300 peak 12672 weight 0.10000E+01 volume 0.77795E+01 ppm1 1.564 ppm2 1.407
ASSI {12712}
( segid "PROT" and resid 115 and name HD1% )
( segid "PROT" and resid 113 and name HB% )
2.300 1.300 1.300 peak 12712 weight 0.10000E+01 volume 0.75629E+01 ppm1 0.752 ppm2 1.412
ASSI {12742}
( segid "PROT" and resid 74 and name HB% )
( segid "PROT" and resid 110 and name HG2% )
2.700 1.800 1.800 peak 12742 weight 0.10000E+01 volume 0.27255E+01 ppm1 6.958 ppm2 0.694
ASSI {12762}
(( segid "PROT" and resid 110 and name HA ))
( segid "PROT" and resid 110 and name HG2% )
2.100 1.100 1.100 peak 12762 weight 0.10000E+01 volume 0.13460E+02 ppm1 3.858 ppm2 0.694
ASSI {12782}
(( segid "PROT" and resid 69 and name HB ))
( segid "PROT" and resid 69 and name HG2% )
2.000 1.000 1.000 peak 12782 weight 0.10000E+01 volume 0.18266E+02 ppm1 2 352 ppm2 0.864
ASSI {12802}
(( segid "PROT" and resid 110 and name HB ))
( segid "PROT" and resid 110 and name HG2% )
2.100 1.100 1.100 peak 12802 weight 0.10000E+01 volume 0.12814E+02 ppm1 1.796 ppm2 0.694
ASSI {12812}
(( segid "PROT" and resid 115 and name HB2 ))
( segid "PROT" and resid 110 and name HG2% )
2.400 1.400 1.400 peak 12812 weight 0.10000E+01 volume 0.58675E+01 ppm1 1.609 ppm2 0.693
ASSI {12822}
(( segid "PROT" and resid 110 and name HG11 ))
( segid "PROT" and resid 110 and name HG2% )
2.400 1.400 1.400 peak 12822 weight 0.10000E+01 volume 0.53638E+01 ppm1 1.154 ppm2 0.692
ASSI {12832}
(( segid "PROT" and resid 110 and name HG12 ))
( segid "PROT" and resid 110 and name HG2% )
2.400 1.400 1.400 peak 12832 weight 0.10000E+01 volume 0.58609E+01 ppm1 1.086 ppm2 0.693
ASSI {12852}
( segid "PROT" and resid 69 and name HG1% )

```

1.0000E+01 volume 0.41193E+02 ppm1 0.986 ppm2 0.861
 0.10000E+01 volume 0.63690E+01 ppm1 7.303 ppm2 1.665
 0.10000E+01 volume 0.37187E+01 ppm1 6.695 ppm2 1.663
 0.10000E+01 volume 0.16636E+01 ppm1 4.399 ppm2 1.531
 0.10000E+01 volume 0.96069E+01 ppm1 4.260 ppm2 1.534
 0.10000E+01 volume 0.52839E+01 ppm1 4.217 ppm2 1.660
 0.10000E+01 volume 0.23966E+02 ppm1 4.116 ppm2 1.534
 0.10000E+01 volume 0.12282E+02 ppm1 3.914 ppm2 1.662
 0.10000E+01 volume 0.58392E+01 ppm1 3.832 ppm2 1.662
 0.10000E+01 volume 0.35679E+01 ppm1 3.416 ppm2 1.662
 0.10000E+01 volume 0.15862E+01 ppm1 1.796 ppm2 1.527
 0.10000E+01 volume 0.42980E+01 ppm1 1.331 ppm2 1.660
 0.10000E+01 volume 0.29370E+01 ppm1 0.163 ppm2 1.664
 0.10000E+01 volume 0.32336E+01 ppm1 4.351 ppm2 1.035
 0.10000E+01 volume 0.26908E+01 ppm1 4.222 ppm2 1.033
 0.10000E+01 volume 0.35525E+01 ppm1 3.979 ppm2 1.031
 0.10000E+01 volume 0.17551E+01 ppm1 1.618 ppm2 0.859
 0.10000E+01 volume 0.41175E+01 ppm1 1.347 ppm2 0.858
 0.10000E+01 volume 0.46372E+01 ppm1 0.568 ppm2 0.861
 0.10000E+01 volume 0.40731E+01 ppm1 7.061 ppm2 1.020
 0.10000E+01 volume 0.97563E+01 ppm1 6.961 ppm2 1.020
 0.10000E+01 volume 0.17544E+01 ppm1 4.152 ppm2 1.016

```

( segid "PROT" and resid 69 and name HG2%)
1.700 0.700 0.700 peak 12852 weight 0.10000E+01 volume 0.41193E+02 ppm1 0.986 ppm2 0.861
ASSI {12872}
(( segid "PROT" and resid 34 and name HZ ))
( segid "PROT" and resid 99 and name HB%)
2.300 1.300 1.300 peak 12872 weight 0.10000E+01 volume 0.63690E+01 ppm1 7.303 ppm2 1.665
ASSI {12882}
( segid "PROT" and resid 82 and name HD%)
( segid "PROT" and resid 99 and name HB%)
2.500 1.600 1.600 peak 12882 weight 0.10000E+01 volume 0.37187E+01 ppm1 6.695 ppm2 1.663
ASSI {12892}
(( segid "PROT" and resid 77 and name HA ))
( segid "PROT" and resid 76 and name HB%)
2.900 2.100 2.100 peak 12892 weight 0.10000E+01 volume 0.16636E+01 ppm1 4.399 ppm2 1.531
ASSI {12902}
(( segid "PROT" and resid 73 and name HA ))
( segid "PROT" and resid 76 and name HB%)
2.200 1.200 1.200 peak 12902 weight 0.10000E+01 volume 0.96069E+01 ppm1 4.260 ppm2 1.534
ASSI {12912}
(( segid "PROT" and resid 82 and name HA ))
( segid "PROT" and resid 99 and name HB%)
2.400 1.400 1.400 peak 12912 weight 0.10000E+01 volume 0.52839E+01 ppm1 4.217 ppm2 1.660
ASSI {12922}
(( segid "PROT" and resid 76 and name HA ))
( segid "PROT" and resid 76 and name HB%)
1.900 0.900 0.900 peak 12922 weight 0.10000E+01 volume 0.23966E+02 ppm1 4.116 ppm2 1.534
ASSI {12932}
(( segid "PROT" and resid 99 and name HA ))
( segid "PROT" and resid 99 and name HB%)
2.100 1.100 1.100 peak 12932 weight 0.10000E+01 volume 0.12282E+02 ppm1 3.914 ppm2 1.662
ASSI {12942}
(( segid "PROT" and resid 96 and name HA ))
( segid "PROT" and resid 99 and name HB%)
2.400 1.400 1.400 peak 12942 weight 0.10000E+01 volume 0.58392E+01 ppm1 3.832 ppm2 1.662
ASSI {12952}
(( segid "PROT" and resid 85 and name HB1 ))
( segid "PROT" and resid 99 and name HB%)
2.600 1.700 1.700 peak 12952 weight 0.10000E+01 volume 0.35679E+01 ppm1 3.416 ppm2 1.662
ASSI {12962}
(( segid "PROT" and resid 80 and name HG1 ))
( segid "PROT" and resid 76 and name HB%)
2.900 2.100 2.100 peak 12962 weight 0.10000E+01 volume 0.15862E+01 ppm1 1.796 ppm2 1.527
ASSI {12972}
(( segid "PROT" and resid 103 and name HB2 ))
( segid "PROT" and resid 99 and name HB%)
2.500 1.600 1.600 peak 12972 weight 0.10000E+01 volume 0.42980E+01 ppm1 1.331 ppm2 1.660
ASSI {12982}
(( segid "PROT" and resid 86 and name HG2 ))
( segid "PROT" and resid 99 and name HB%)
2.700 1.800 1.800 peak 12982 weight 0.10000E+01 volume 0.29370E+01 ppm1 0.163 ppm2 1.664
ASSI {13002}
(( segid "PROT" and resid 30 and name HB1 ))
( segid "PROT" and resid 101 and name HG2%)
2.600 1.700 1.700 peak 13002 weight 0.10000E+01 volume 0.32336E+01 ppm1 4.351 ppm2 1.035
ASSI {13022}
(( segid "PROT" and resid 98 and name HA ))
( segid "PROT" and resid 101 and name HG2%)
2.700 1.800 1.800 peak 13022 weight 0.10000E+01 volume 0.26908E+01 ppm1 4.222 ppm2 1.033
ASSI {13032}
(( segid "PROT" and resid 30 and name HB2 ))
( segid "PROT" and resid 101 and name HG2%)
2.600 1.700 1.700 peak 13032 weight 0.10000E+01 volume 0.35525E+01 ppm1 3.979 ppm2 1.031
ASSI {13072}
(( segid "PROT" and resid 115 and name HB2 ))
( segid "PROT" and resid 116 and name HG2%)
2.900 2.100 2.100 peak 13072 weight 0.10000E+01 volume 0.17551E+01 ppm1 1.618 ppm2 0.859
ASSI {13082}
(( segid "PROT" and resid 116 and name HG11))
( segid "PROT" and resid 116 and name HG2%)
2.500 1.600 1.600 peak 13082 weight 0.10000E+01 volume 0.41175E+01 ppm1 1.347 ppm2 0.858
ASSI {13092}
( segid "PROT" and resid 110 and name HD1%)
( segid "PROT" and resid 116 and name HG2%)
2.500 1.600 1.600 peak 13092 weight 0.10000E+01 volume 0.46372E+01 ppm1 0.568 ppm2 0.861
ASSI {13102}
(( segid "PROT" and resid 24 and name HE21))
( segid "PROT" and resid 21 and name HG2%)
2.500 1.600 1.600 peak 13102 weight 0.10000E+01 volume 0.40731E+01 ppm1 7.061 ppm2 1.020
ASSI {13112}
( segid "PROT" and resid 106 and name HD%)
( segid "PROT" and resid 21 and name HG2%)
2.200 1.200 1.200 peak 13112 weight 0.10000E+01 volume 0.97563E+01 ppm1 6.961 ppm2 1.020
ASSI {13122}
(( segid "PROT" and resid 22 and name HA ))
( segid "PROT" and resid 21 and name HG2%)
2.900 2.100 2.100 peak 13122 weight 0.10000E+01 volume 0.17544E+01 ppm1 4.152 ppm2 1.016
ASSI {13132}
(( segid "PROT" and resid 21 and name HA ))
( segid "PROT" and resid 21 and name HG2%)

```

2.200	1.200	1.200	peak 13132	weight	0.10000E+01	volume	0.82544E+01	ppm1	3.800	ppm2	1.019
ASSI {13142}											
((segid "PROT" and resid 18 and name HA))											
(segid "PROT" and resid 21 and name HG2%)											
2.900	2.100	2.100	peak 13142	weight	0.10000E+01	volume	0.16321E+01	ppm1	3.319	ppm2	1.017
ASSI {13162}											
((segid "PROT" and resid 21 and name HG11))											
(segid "PROT" and resid 21 and name HG2%)											
2.300	1.300	1.300	peak 13162	weight	0.10000E+01	volume	0.61393E+01	ppm1	1.785	ppm2	1.018
ASSI {13202}											
(segid "PROT" and resid 78 and name HD2%)											
(segid "PROT" and resid 21 and name HG2%)											
2.900	2.100	2.100	peak 13202	weight	0.10000E+01	volume	0.15853E+01	ppm1	0.196	ppm2	1.016
ASSI {13212}											
(segid "PROT" and resid 78 and name HD1%)											
(segid "PROT" and resid 21 and name HG2%)											
2.700	1.800	1.800	peak 13212	weight	0.10000E+01	volume	0.24623E+01	ppm1	0.093	ppm2	1.018
ASSI {13292}											
((segid "PROT" and resid 75 and name HB1))											
(segid "PROT" and resid 75 and name HE%)											
2.700	1.800	1.800	peak 13292	weight	0.10000E+01	volume	0.24960E+01	ppm1	2.964	ppm2	2.093
ASSI {13322}											
((segid "PROT" and resid 75 and name HG1))											
(segid "PROT" and resid 75 and name HE%)											
2.400	1.400	1.400	peak 13322	weight	0.10000E+01	volume	0.47718E+01	ppm1	2.353	ppm2	2.090
ASSI {13332}											
((segid "PROT" and resid 75 and name HG2))											
(segid "PROT" and resid 75 and name HE%)											
2.400	1.400	1.400	peak 13332	weight	0.10000E+01	volume	0.50489E+01	ppm1	2.245	ppm2	2.089
ASSI {13342}											
((segid "PROT" and resid 115 and name HB2))											
(segid "PROT" and resid 75 and name HE%)											
2.700	1.800	1.800	peak 13342	weight	0.10000E+01	volume	0.25149E+01	ppm1	1.610	ppm2	2.097
ASSI {13362}											
(segid "PROT" and resid 116 and name HG2%)											
(segid "PROT" and resid 75 and name HE%)											
2.500	1.600	1.600	peak 13362	weight	0.10000E+01	volume	0.44297E+01	ppm1	0.848	ppm2	2.096
ASSI {13372}											
(segid "PROT" and resid 115 and name HD1%)											
(segid "PROT" and resid 75 and name HE%)											
2.600	1.700	1.700	peak 13372	weight	0.10000E+01	volume	0.32468E+01	ppm1	0.752	ppm2	2.096
ASSI {13382}											
(segid "PROT" and resid 110 and name HG2%)											
(segid "PROT" and resid 75 and name HE%)											
2.400	1.400	1.400	peak 13382	weight	0.10000E+01	volume	0.50045E+01	ppm1	0.691	ppm2	2.096
ASSI {13392}											
(segid "PROT" and resid 110 and name HD1%)											
(segid "PROT" and resid 75 and name HE%)											
2.400	1.400	1.400	peak 13392	weight	0.10000E+01	volume	0.54701E+01	ppm1	0.579	ppm2	2.094
ASSI {13402}											
((segid "PROT" and resid 32 and name HA))											
(segid "PROT" and resid 35 and name HE%)											
2.700	1.800	1.800	peak 13402	weight	0.10000E+01	volume	0.26368E+01	ppm1	4.426	ppm2	2.218
ASSI {13412}											
((segid "PROT" and resid 35 and name HA))											
(segid "PROT" and resid 35 and name HE%)											
2.700	1.800	1.800	peak 13412	weight	0.10000E+01	volume	0.23762E+01	ppm1	4.340	ppm2	2.215
ASSI {13422}											
((segid "PROT" and resid 26 and name HA))											
(segid "PROT" and resid 35 and name HE%)											
2.800	2.000	2.000	peak 13422	weight	0.10000E+01	volume	0.21502E+01	ppm1	3.936	ppm2	2.227
ASSI {13432}											
((segid "PROT" and resid 35 and name HG1))											
(segid "PROT" and resid 35 and name HE%)											
2.200	1.200	1.200	peak 13432	weight	0.10000E+01	volume	0.99990E+01	ppm1	2.894	ppm2	2.218
ASSI {13442}											
((segid "PROT" and resid 35 and name HB1))											
(segid "PROT" and resid 35 and name HE%)											
2.400	1.400	1.400	peak 13442	weight	0.10000E+01	volume	0.60108E+01	ppm1	2.319	ppm2	2.207
ASSI {13452}											
((segid "PROT" and resid 26 and name HB1))											
(segid "PROT" and resid 35 and name HE%)											
2.400	2.400	2.100	peak 13452	weight	0.10000E+01	volume	0.47279E+01	ppm1	1.919	ppm2	2.220
ASSI {13482}											
((segid "PROT" and resid 26 and name HG1))											
(segid "PROT" and resid 35 and name HE%)											
2.900	2.100	2.100	peak 13482	weight	0.10000E+01	volume	0.17649E+01	ppm1	1.532	ppm2	2.221
ASSI {13542}											
((segid "PROT" and resid 84 and name HA))											
(segid "PROT" and resid 50 and name HG2%)											
2.800	2.000	2.000	peak 13542	weight	0.10000E+01	volume	0.19891E+01	ppm1	4.343	ppm2	0.420
ASSI {13552}											
((segid "PROT" and resid 59 and name HA))											
(segid "PROT" and resid 59 and name HE%)											
2.800	2.000	2.000	peak 13552	weight	0.10000E+01	volume	0.20245E+01	ppm1	4.337	ppm2	1.307
ASSI {13562}											
((segid "PROT" and resid 53 and name HA))											
(segid "PROT" and resid 50 and name HG2%)											
2.200	1.200	1.200	peak 13562	weight	0.10000E+01	volume	0.82735E+01	ppm1	4.125	ppm2	0.419

```

ASSI {13572}
(( segid "PROT" and resid 50 and name HA ))
( segid "PROT" and resid 50 and name HG2%)
2.200 1.200 1.200 peak 13572 weight 0.10000E+01 volume 0.79741E+01 ppm1 3.953 ppm2 0.421
ASSI {13582}
(( segid "PROT" and resid 74 and name HA ))
( segid "PROT" and resid 59 and name HE%)
2.700 1.800 1.800 peak 13582 weight 0.10000E+01 volume 0.25189E+01 ppm1 3.803 ppm2 1.311
ASSI {13592}
(( segid "PROT" and resid 53 and name HD2 ))
( segid "PROT" and resid 50 and name HG2%)
2.800 2.000 2.000 peak 13592 weight 0.10000E+01 volume 0.20585E+01 ppm1 3.445 ppm2 0.420
ASSI {13612}
(( segid "PROT" and resid 84 and name HB1 ))
( segid "PROT" and resid 50 and name HG2%)
2.700 1.800 1.800 peak 13612 weight 0.10000E+01 volume 0.27693E+01 ppm1 3.035 ppm2 0.417
ASSI {13622}
(( segid "PROT" and resid 77 and name HB1 ))
( segid "PROT" and resid 59 and name HE%)
2.300 1.300 1.300 peak 13622 weight 0.10000E+01 volume 0.75013E+01 ppm1 2.753 ppm2 1.308
ASSI {13632}
(( segid "PROT" and resid 84 and name HB2 ))
( segid "PROT" and resid 50 and name HG2%)
2.700 1.800 1.800 peak 13632 weight 0.10000E+01 volume 0.28676E+01 ppm1 2.712 ppm2 0.420
ASSI {13642}
(( segid "PROT" and resid 59 and name HG2 ))
( segid "PROT" and resid 59 and name HE%)
2.600 1.700 1.700 peak 13642 weight 0.10000E+01 volume 0.33032E+01 ppm1 2.560 ppm2 1.310
ASSI {13652}
(( segid "PROT" and resid 53 and name HB1 ))
( segid "PROT" and resid 50 and name HG2%)
2.600 1.700 1.700 peak 13652 weight 0.10000E+01 volume 0.34701E+01 ppm1 2.259 ppm2 0.419
ASSI {13662}
(( segid "PROT" and resid 59 and name HB1 ))
( segid "PROT" and resid 59 and name HE%)
2.400 1.400 1.400 peak 13662 weight 0.10000E+01 volume 0.54884E+01 ppm1 2.154 ppm2 1.309
ASSI {13672}
(( segid "PROT" and resid 59 and name HB2 ))
( segid "PROT" and resid 59 and name HE%)
2.500 1.600 1.600 peak 13672 weight 0.10000E+01 volume 0.41611E+01 ppm1 1.932 ppm2 1.309
ASSI {13682}
(( segid "PROT" and resid 53 and name HG2 ))
( segid "PROT" and resid 50 and name HG2%)
2.600 1.700 1.700 peak 13682 weight 0.10000E+01 volume 0.31884E+01 ppm1 1.934 ppm2 0.421
ASSI {13692}
(( segid "PROT" and resid 50 and name HB ))
( segid "PROT" and resid 50 and name HG2%)
2.100 1.100 1.100 peak 13692 weight 0.10000E+01 volume 0.11042E+02 ppm1 1.250 ppm2 0.421
ASSI {13712}
(( segid "PROT" and resid 50 and name HG11))
( segid "PROT" and resid 50 and name HG2%)
2.500 1.600 1.600 peak 13712 weight 0.10000E+01 volume 0.37929E+01 ppm1 0.830 ppm2 0.420
ASSI {13722}
(( segid "PROT" and resid 78 and name HG ))
( segid "PROT" and resid 59 and name HE%)
2.500 1.600 1.600 peak 13722 weight 0.10000E+01 volume 0.39705E+01 ppm1 0.704 ppm2 1.311
ASSI {13732}
( segid "PROT" and resid 50 and name HD1%)
( segid "PROT" and resid 50 and name HG2%)
2.000 1.000 1.000 peak 13732 weight 0.10000E+01 volume 0.14950E+02 ppm1 0.581 ppm2 0.419
ASSI {13742}
(( segid "PROT" and resid 78 and name HB2 ))
( segid "PROT" and resid 59 and name HE%)
2.400 1.400 1.400 peak 13742 weight 0.10000E+01 volume 0.56802E+01 ppm1 0.475 ppm2 1.310
ASSI {13762}
(( segid "PROT" and resid 50 and name HG12))
( segid "PROT" and resid 50 and name HG2%)
2.400 1.400 1.400 peak 13762 weight 0.10000E+01 volume 0.49893E+01 ppm1 0.188 ppm2 0.422
ASSI {13782}
(( segid "PROT" and resid 54 and name HA ))
( segid "PROT" and resid 54 and name HE%)
2.200 1.200 1.200 peak 13782 weight 0.10000E+01 volume 0.96092E+01 ppm1 4.986 ppm2 2.003
ASSI {13792}
(( segid "PROT" and resid 77 and name HA ))
( segid "PROT" and resid 54 and name HE%)
2.900 2.100 2.100 peak 13792 weight 0.10000E+01 volume 0.17796E+01 ppm1 4.395 ppm2 2.006
ASSI {13802}
(( segid "PROT" and resid 54 and name HG1 ))
( segid "PROT" and resid 54 and name HE%)
2.400 1.400 1.400 peak 13802 weight 0.10000E+01 volume 0.54019E+01 ppm1 2.742 ppm2 2.001
ASSI {13812}
(( segid "PROT" and resid 54 and name HB2 ))
( segid "PROT" and resid 54 and name HE%)
2.500 1.600 1.600 peak 13812 weight 0.10000E+01 volume 0.37957E+01 ppm1 1.383 ppm2 2.004
ASSI {13832}
( segid "PROT" and resid 81 and name HG1%)
( segid "PROT" and resid 54 and name HE%)
2.700 1.800 1.800 peak 13832 weight 0.10000E+01 volume 0.24284E+01 ppm1 0.510 ppm2 2.002
ASSI {13852}

```



```

(( segid "PROT" and resid 98 and name HA ))
( segid "PROT" and resid 101 and name HD1%)
2.400 1.400 1.400 peak 13852 weight 0.10000E+01 volume 0.57589E+01 ppm1 4.226 ppm2 0.997
ASSI {13862}
(( segid "PROT" and resid 101 and name HA ))
( segid "PROT" and resid 101 and name HD1%)
2.500 1.600 1.600 peak 13862 weight 0.10000E+01 volume 0.41504E+01 ppm1 3.695 ppm2 1.001
ASSI {13872}
(( segid "PROT" and resid 18 and name HA ))
( segid "PROT" and resid 21 and name HD1%)
2.600 1.700 1.700 peak 13872 weight 0.10000E+01 volume 0.31541E+01 ppm1 3.312 ppm2 0.653
ASSI {13892}
(( segid "PROT" and resid 97 and name HB1 ))
( segid "PROT" and resid 101 and name HD1%)
2.800 2.000 2.000 peak 13892 weight 0.10000E+01 volume 0.19889E+01 ppm1 2.112 ppm2 0.993
ASSI {13902}
(( segid "PROT" and resid 21 and name HB ))
( segid "PROT" and resid 21 and name HD1%)
2.300 1.300 1.300 peak 13902 weight 0.10000E+01 volume 0.69789E+01 ppm1 1.951 ppm2 0.652
ASSI {13912}
(( segid "PROT" and resid 101 and name HG11))
( segid "PROT" and resid 101 and name HD1%)
2.000 1.000 1.000 peak 13912 weight 0.10000E+01 volume 0.16613E+02 ppm1 1.897 ppm2 0.998
ASSI {13922}
(( segid "PROT" and resid 21 and name HG11))
( segid "PROT" and resid 21 and name HD1%)
2.100 1.100 1.100 peak 13922 weight 0.10000E+01 volume 0.12244E+02 ppm1 1.786 ppm2 0.651
ASSI {13932}
(( segid "PROT" and resid 109 and name HB2 ))
( segid "PROT" and resid 21 and name HD1%)
2.600 1.700 1.700 peak 13932 weight 0.10000E+01 volume 0.35134E+01 ppm1 1.581 ppm2 0.646
ASSI {13942}
( segid "PROT" and resid 113 and name HB%)
( segid "PROT" and resid 21 and name HD1%)
2.100 1.100 1.100 peak 13942 weight 0.10000E+01 volume 0.12667E+02 ppm1 1.411 ppm2 0.651
ASSI {13952}
(( segid "PROT" and resid 101 and name HG12))
( segid "PROT" and resid 101 and name HD1%)
2.000 1.000 1.000 peak 13952 weight 0.10000E+01 volume 0.17265E+02 ppm1 1.239 ppm2 0.997
ASSI {13972}
( segid "PROT" and resid 21 and name HG2%)
( segid "PROT" and resid 21 and name HD1%)
1.900 0.900 0.900 peak 13972 weight 0.10000E+01 volume 0.21366E+02 ppm1 1.024 ppm2 0.651
ASSI {13992}
( segid "PROT" and resid 106 and name HD%)
( segid "PROT" and resid 110 and name HD1%)
2.800 2.000 2.000 peak 13992 weight 0.10000E+01 volume 0.21957E+01 ppm1 6.962 ppm2 0.566
ASSI {14002}
(( segid "PROT" and resid 116 and name HA ))
( segid "PROT" and resid 116 and name HD1%)
2.500 1.600 1.600 peak 14002 weight 0.10000E+01 volume 0.37164E+01 ppm1 4.274 ppm2 0.829
ASSI {14012}
(( segid "PROT" and resid 75 and name HA ))
( segid "PROT" and resid 116 and name HD1%)
2.800 2.000 2.000 peak 14012 weight 0.10000E+01 volume 0.22585E+01 ppm1 4.096 ppm2 0.828
ASSI {14052}
( segid "PROT" and resid 75 and name HE%)
( segid "PROT" and resid 116 and name HD1%)
2.700 1.800 1.800 peak 14052 weight 0.10000E+01 volume 0.23966E+01 ppm1 2.095 ppm2 0.826
ASSI {14082}
(( segid "PROT" and resid 6 and name HD1 ))
( segid "PROT" and resid 116 and name HD1%)
2.900 2.100 2.100 peak 14082 weight 0.10000E+01 volume 0.18157E+01 ppm1 1.663 ppm2 0.826
ASSI {14092}
(( segid "PROT" and resid 115 and name HB2 ))
( segid "PROT" and resid 110 and name HD1%)
2.600 1.700 1.700 peak 14092 weight 0.10000E+01 volume 0.33126E+01 ppm1 1.602 ppm2 0.575
ASSI {14102}
(( segid "PROT" and resid 116 and name HG11))
( segid "PROT" and resid 116 and name HD1%)
2.100 1.100 1.100 peak 14102 weight 0.10000E+01 volume 0.13147E+02 ppm1 1.345 ppm2 0.826
ASSI {14112}
(( segid "PROT" and resid 110 and name HG11))
( segid "PROT" and resid 110 and name HD1%)
2.200 1.200 1.200 peak 14112 weight 0.10000E+01 volume 0.10025E+02 ppm1 1.157 ppm2 0.578
ASSI {14132}
(( segid "PROT" and resid 110 and name HG12))
( segid "PROT" and resid 110 and name HD1%)
2.100 1.100 1.100 peak 14132 weight 0.10000E+01 volume 0.11467E+02 ppm1 1.088 ppm2 0.578
ASSI {14142}
(( segid "PROT" and resid 116 and name HG12))
( segid "PROT" and resid 116 and name HD1%)
2.000 1.000 1.000 peak 14142 weight 0.10000E+01 volume 0.15573E+02 ppm1 0.961 ppm2 0.825
ASSI {14152}
( segid "PROT" and resid 116 and name HD1%)
( segid "PROT" and resid 110 and name HD1%)
2.300 1.300 1.300 peak 14152 weight 0.10000E+01 volume 0.75073E+01 ppm1 0.844 ppm2 0.569
ASSI {14212}
(( segid "PROT" and resid 84 and name HA ))

```

```

( segid "PROT" and resid 50 and name HD1%)
2.200 1.200 1.200 peak 14212 weight 0.10000E+01 volume 0.81666E+01 ppm1 4.342 ppm2 0.580
ASSI {14222}
(( segid "PROT" and resid 53 and name HA ))
( segid "PROT" and resid 50 and name HD1%)
2.900 2.100 2.100 peak 14222 weight 0.10000E+01 volume 0.16892E+01 ppm1 4.122 ppm2 0.584
ASSI {14242}
(( segid "PROT" and resid 84 and name HB1 ))
( segid "PROT" and resid 50 and name HD1%)
2.500 1.600 1.600 peak 14242 weight 0.10000E+01 volume 0.45606E+01 ppm1 3.035 ppm2 0.580
ASSI {14252}
(( segid "PROT" and resid 88 and name HB1 ))
( segid "PROT" and resid 50 and name HD1%)
2.600 1.700 1.700 peak 14252 weight 0.10000E+01 volume 0.34453E+01 ppm1 2.949 ppm2 0.582
ASSI {14262}
(( segid "PROT" and resid 84 and name HB2 ))
( segid "PROT" and resid 50 and name HD1%)
2.700 1.800 1.800 peak 14262 weight 0.10000E+01 volume 0.24442E+01 ppm1 2.714 ppm2 0.580
ASSI {14272}
(( segid "PROT" and resid 87 and name HB1 ))
( segid "PROT" and resid 50 and name HD1%)
2.500 1.600 1.600 peak 14272 weight 0.10000E+01 volume 0.41877E+01 ppm1 2.234 ppm2 0.583
ASSI {14282}
(( segid "PROT" and resid 87 and name HB2 ))
( segid "PROT" and resid 50 and name HD1%)
2.600 1.700 1.700 peak 14282 weight 0.10000E+01 volume 0.30054E+01 ppm1 2.059 ppm2 0.581
ASSI {14292}
(( segid "PROT" and resid 50 and name HB ))
( segid "PROT" and resid 50 and name HD1%)
2.500 1.600 1.600 peak 14292 weight 0.10000E+01 volume 0.43255E+01 ppm1 1.249 ppm2 0.580
ASSI {14302}
( segid "PROT" and resid 49 and name HG1%)
( segid "PROT" and resid 50 and name HD1%)
2.400 1.400 1.400 peak 14302 weight 0.10000E+01 volume 0.48009E+01 ppm1 0.954 ppm2 0.580
ASSI {14322}
(( segid "PROT" and resid 50 and name HG11))
( segid "PROT" and resid 50 and name HD1%)
2.200 1.200 1.200 peak 14322 weight 0.10000E+01 volume 0.93672E+01 ppm1 0.834 ppm2 0.582
ASSI {14342}
(( segid "PROT" and resid 50 and name HG12))
( segid "PROT" and resid 50 and name HD1%)
2.200 1.200 1.200 peak 14342 weight 0.10000E+01 volume 0.83520E+01 ppm1 0.190 ppm2 0.583
ASSI {14352}
(( segid "PROT" and resid 6 and name HD1 ))
(( segid "PROT" and resid 6 and name HA ))
2.400 1.400 1.400 peak 14352 weight 0.10000E+01 volume 0.48806E+01 ppm1 1.680 ppm2 4.375
ASSI {14382}
(( segid "PROT" and resid 7 and name HG1 ))
(( segid "PROT" and resid 7 and name HB1 ))
1.800 0.800 0.800 peak 14382 weight 0.10000E+01 volume 0.31365E+02 ppm1 2.308 ppm2 2.086
ASSI {14422}
(( segid "PROT" and resid 61 and name HB2 ))
(( segid "PROT" and resid 61 and name HA ))
2.000 1.000 1.000 peak 14422 weight 0.10000E+01 volume 0.15249E+02 ppm1 2.101 ppm2 4.084
ASSI {14462}
(( segid "PROT" and resid 92 and name HG2 ))
(( segid "PROT" and resid 92 and name HG1 ))
1.700 0.700 0.700 peak 14462 weight 0.10000E+01 volume 0.36116E+02 ppm1 2.266 ppm2 2.386
ASSI {14472}
(( segid "PROT" and resid 94 and name HA ))
(( segid "PROT" and resid 94 and name HB2 ))
2.300 1.300 1.300 peak 14472 weight 0.10000E+01 volume 0.67398E+01 ppm1 4.244 ppm2 2.035
ASSI {14542}
( segid "PROT" and resid 41 and name HG2%)
(( segid "PROT" and resid 41 and name HA ))
2.200 1.200 1.200 peak 14542 weight 0.10000E+01 volume 0.86782E+01 ppm1 1.318 ppm2 4.097
ASSI {14582}
(( segid "PROT" and resid 30 and name HA ))
(( segid "PROT" and resid 30 and name HB1 ))
3.100 2.400 2.400 peak 14582 weight 0.10000E+01 volume 0.12468E+01 ppm1 4.854 ppm2 4.344
ASSI {14632}
(( segid "PROT" and resid 89 and name HB2 ))
(( segid "PROT" and resid 89 and name HB1 ))
2.400 1.400 1.400 peak 14632 weight 0.10000E+01 volume 0.59384E+01 ppm1 2.904 ppm2 3.100
ASSI {14642}
(( segid "PROT" and resid 10 and name HA ))
(( segid "PROT" and resid 10 and name HB2 ))
2.500 1.600 1.600 peak 14642 weight 0.10000E+01 volume 0.42768E+01 ppm1 4.918 ppm2 2.734
ASSI {14652}
(( segid "PROT" and resid 12 and name HA ))
(( segid "PROT" and resid 12 and name HB2 ))
2.500 1.600 1.600 peak 14652 weight 0.10000E+01 volume 0.46107E+01 ppm1 4.723 ppm2 2.794
ASSI {14692}
(( segid "PROT" and resid 13 and name HG2 ))
(( segid "PROT" and resid 13 and name HA ))
2.300 1.300 1.300 peak 14692 weight 0.10000E+01 volume 0.67869E+01 ppm1 2.430 ppm2 4.217
ASSI {14722}
(( segid "PROT" and resid 20 and name HA ))
(( segid "PROT" and resid 23 and name HG1 ))

```

3.000	2.200	2.200	peak 14722	weight	0.10000E+01	volume	0.12728E+01	ppm1	4.319	ppm2	2.575
ASSI {14732}											
((segid "PROT" and resid 20 and name HA))											
((segid "PROT" and resid 23 and name HG2))											
3.100	2.400	2.400	peak 14732	weight	0.10000E+01	volume	0.10567E+01	ppm1	4.319	ppm2	2.482
ASSI {14782}											
((segid "PROT" and resid 23 and name HB2))											
((segid "PROT" and resid 23 and name HA))											
2.100	1.100	1.100	peak 14782	weight	0.10000E+01	volume	0.12638E+02	ppm1	2.272	ppm2	4.078
ASSI {14802}											
((segid "PROT" and resid 23 and name HG2))											
((segid "PROT" and resid 23 and name HB2))											
2.100	1.100	1.100	peak 14802	weight	0.10000E+01	volume	0.11531E+02	ppm1	2.492	ppm2	2.247
ASSI {14822}											
((segid "PROT" and resid 24 and name HB2))											
((segid "PROT" and resid 24 and name HA))											
2.300	1.300	1.300	peak 14822	weight	0.10000E+01	volume	0.73231E+01	ppm1	2.421	ppm2	4.227
ASSI {14842}											
((segid "PROT" and resid 24 and name HG1))											
((segid "PROT" and resid 24 and name HB2))											
2.700	1.800	1.800	peak 14842	weight	0.10000E+01	volume	0.29089E+01	ppm1	2.891	ppm2	2.418
ASSI {14852}											
((segid "PROT" and resid 21 and name HA))											
((segid "PROT" and resid 24 and name HG1))											
3.200	2.600	2.300	peak 14852	weight	0.10000E+01	volume	0.98750E+00	ppm1	3.800	ppm2	2.889
ASSI {14862}											
((segid "PROT" and resid 29 and name HG1))											
((segid "PROT" and resid 29 and name HA))											
2.300	1.300	1.300	peak 14862	weight	0.10000E+01	volume	0.65450E+01	ppm1	2.506	ppm2	4.225
ASSI {14912}											
((segid "PROT" and resid 79 and name HB1))											
((segid "PROT" and resid 79 and name HG1))											
2.100	1.100	1.100	peak 14912	weight	0.10000E+01	volume	0.13602E+02	ppm1	2.216	ppm2	2.463
ASSI {14922}											
((segid "PROT" and resid 79 and name HB2))											
((segid "PROT" and resid 79 and name HG1))											
2.100	1.100	1.100	peak 14922	weight	0.10000E+01	volume	0.11814E+02	ppm1	2.118	ppm2	2.465
ASSI {14932}											
((segid "PROT" and resid 56 and name HG))											
((segid "PROT" and resid 34 and name HB1))											
3.000	2.200	2.200	peak 14932	weight	0.10000E+01	volume	0.14093E+01	ppm1	1.768	ppm2	3.519
ASSI {14962}											
((segid "PROT" and resid 56 and name HG))											
((segid "PROT" and resid 34 and name HB2))											
3.100	2.400	2.400	peak 14962	weight	0.10000E+01	volume	0.10685E+01	ppm1	1.761	ppm2	2.631
ASSI {14982}											
((segid "PROT" and resid 53 and name HG1))											
((segid "PROT" and resid 52 and name HA))											
3.100	2.400	2.400	peak 14982	weight	0.10000E+01	volume	0.11187E+01	ppm1	2.273	ppm2	5.037
ASSI {15012}											
((segid "PROT" and resid 82 and name HB2))											
((segid "PROT" and resid 82 and name HA))											
2.600	1.700	1.700	peak 15012	weight	0.10000E+01	volume	0.29905E+01	ppm1	3.033	ppm2	4.215
ASSI {15052}											
((segid "PROT" and resid 102 and name HD2%))											
((segid "PROT" and resid 106 and name HB2))											
2.900	2.100	2.100	peak 15052	weight	0.10000E+01	volume	0.16469E+01	ppm1	0.767	ppm2	3.138
ASSI {15072}											
((segid "PROT" and resid 18 and name HB1))											
((segid "PROT" and resid 15 and name HA))											
3.000	2.200	2.200	peak 15072	weight	0.10000E+01	volume	0.12939E+01	ppm1	1.550	ppm2	4.042
ASSI {15092}											
((segid "PROT" and resid 62 and name HA))											
((segid "PROT" and resid 67 and name HB2))											
3.100	2.400	2.400	peak 15092	weight	0.10000E+01	volume	0.11858E+01	ppm1	3.919	ppm2	2.090
ASSI {15102}											
((segid "PROT" and resid 68 and name HB1))											
((segid "PROT" and resid 68 and name HA))											
3.100	2.400	2.400	peak 15102	weight	0.10000E+01	volume	0.11603E+01	ppm1	3.114	ppm2	4.581
ASSI {15132}											
((segid "PROT" and resid 62 and name HB2))											
((segid "PROT" and resid 68 and name HB2))											
3.300	2.700	2.200	peak 15132	weight	0.10000E+01	volume	0.82400E+00	ppm1	1.080	ppm2	2.966
ASSI {15142}											
((segid "PROT" and resid 62 and name HB2))											
((segid "PROT" and resid 68 and name HB1))											
3.300	2.700	2.200	peak 15142	weight	0.10000E+01	volume	0.85460E+00	ppm1	1.077	ppm2	3.106
ASSI {15162}											
((segid "PROT" and resid 57 and name HB1))											
((segid "PROT" and resid 57 and name HA))											
3.300	2.700	2.200	peak 15162	weight	0.10000E+01	volume	0.86210E+00	ppm1	2.603	ppm2	3.909
ASSI {15172}											
((segid "PROT" and resid 28 and name HB1))											
((segid "PROT" and resid 28 and name HA))											
2.600	1.700	1.700	peak 15172	weight	0.10000E+01	volume	0.30616E+01	ppm1	3.016	ppm2	4.021
ASSI {15212}											
((segid "PROT" and resid 28 and name HB2))											
((segid "PROT" and resid 25 and name HA))											
3.100	2.400	2.400	peak 15212	weight	0.10000E+01	volume	0.12595E+01	ppm1	2.817	ppm2	3.868

```

ASSI {15242}
  ( segid "PROT" and resid 25 and name HG2% )
  ( ( segid "PROT" and resid 25 and name HA ) )
  2.300 1.300 1.300 peak 15242 weight 0.10000E+01 volume 0.70013E+01 ppm1 1.069 ppm2 3.871
ASSI {15262}
  ( ( segid "PROT" and resid 106 and name HB1 ) )
  ( segid "PROT" and resid 25 and name HG1% )
  3.200 2.600 2.300 peak 15262 weight 0.10000E+01 volume 0.94350E+00 ppm1 3.357 ppm2 1.244
ASSI {15292}
  ( ( segid "PROT" and resid 37 and name HA ) )
  ( segid "PROT" and resid 38 and name HG1% )
  3.200 2.600 2.300 peak 15292 weight 0.10000E+01 volume 0.10144E+01 ppm1 4.278 ppm2 0.489
ASSI {15302}
  ( ( segid "PROT" and resid 55 and name HB1 ) )
  ( segid "PROT" and resid 81 and name HG1% )
  3.000 2.200 2.200 peak 15302 weight 0.10000E+01 volume 0.14883E+01 ppm1 2.400 ppm2 0.506
ASSI {15322}
  ( ( segid "PROT" and resid 43 and name HA ) )
  ( segid "PROT" and resid 38 and name HG2% )
  3.000 2.200 2.200 peak 15322 weight 0.10000E+01 volume 0.12695E+01 ppm1 4.983 ppm2 -0.010
ASSI {15432}
  ( ( segid "PROT" and resid 82 and name HA ) )
  ( segid "PROT" and resid 81 and name HG2% )
  3.000 2.200 2.200 peak 15432 weight 0.10000E+01 volume 0.14427E+01 ppm1 4.218 ppm2 0.155
ASSI {15452}
  ( ( segid "PROT" and resid 33 and name HG2 ) )
  ( ( segid "PROT" and resid 33 and name HA ) )
  3.200 2.600 2.300 peak 15452 weight 0.10000E+01 volume 0.88590E+00 ppm1 -0.871 ppm2 3.994
ASSI {15462}
  ( ( segid "PROT" and resid 33 and name HB1 ) )
  ( ( segid "PROT" and resid 33 and name HA ) )
  3.000 2.200 2.200 peak 15462 weight 0.10000E+01 volume 0.12852E+01 ppm1 1.064 ppm2 3.985
ASSI {15472}
  ( ( segid "PROT" and resid 14 and name HB2 ) )
  ( ( segid "PROT" and resid 14 and name HA ) )
  2.500 1.600 1.600 peak 15472 weight 0.10000E+01 volume 0.41749E+01 ppm1 1.597 ppm2 4.090
ASSI {15482}
  ( ( segid "PROT" and resid 14 and name HB1 ) )
  ( ( segid "PROT" and resid 14 and name HA ) )
  2.200 1.200 1.200 peak 15482 weight 0.10000E+01 volume 0.79299E+01 ppm1 1.913 ppm2 4.085
ASSI {15502}
  ( segid "PROT" and resid 17 and name HG2% )
  ( ( segid "PROT" and resid 14 and name HA ) )
  3.100 2.400 2.400 peak 15502 weight 0.10000E+01 volume 0.11760E+01 ppm1 1.179 ppm2 4.098
ASSI {15512}
  ( ( segid "PROT" and resid 11 and name HA ) )
  ( ( segid "PROT" and resid 14 and name HB2 ) )
  3.000 2.200 2.200 peak 15512 weight 0.10000E+01 volume 0.13340E+01 ppm1 4.372 ppm2 1.592
ASSI {15522}
  ( ( segid "PROT" and resid 70 and name HN ) )
  ( ( segid "PROT" and resid 14 and name HG ) )
  3.100 2.400 2.400 peak 15522 weight 0.10000E+01 volume 0.10950E+01 ppm1 7.488 ppm2 1.424
ASSI {15542}
  ( ( segid "PROT" and resid 70 and name HA ) )
  ( segid "PROT" and resid 14 and name HD2% )
  3.100 2.400 2.400 peak 15542 weight 0.10000E+01 volume 0.11378E+01 ppm1 4.807 ppm2 0.833
ASSI {15552}
  ( ( segid "PROT" and resid 18 and name HB1 ) )
  ( ( segid "PROT" and resid 18 and name HA ) )
  2.800 2.000 2.000 peak 15552 weight 0.10000E+01 volume 0.22536E+01 ppm1 1.562 ppm2 3.316
ASSI {15562}
  ( segid "PROT" and resid 17 and name HG2% )
  ( ( segid "PROT" and resid 18 and name HA ) )
  3.000 2.200 2.200 peak 15562 weight 0.10000E+01 volume 0.14142E+01 ppm1 1.178 ppm2 3.312
ASSI {15572}
  ( ( segid "PROT" and resid 21 and name HG12 ) )
  ( segid "PROT" and resid 18 and name HA )
  3.000 2.200 2.200 peak 15572 weight 0.10000E+01 volume 0.14946E+01 ppm1 1.071 ppm2 3.312
ASSI {15592}
  ( ( segid "PROT" and resid 18 and name HB2 ) )
  ( ( segid "PROT" and resid 18 and name HA ) )
  2.700 1.800 1.800 peak 15592 weight 0.10000E+01 volume 0.26695E+01 ppm1 0.342 ppm2 3.314
ASSI {15642}
  ( ( segid "PROT" and resid 18 and name HG ) )
  ( ( segid "PROT" and resid 18 and name HB2 ) )
  3.100 2.400 2.400 peak 15642 weight 0.10000E+01 volume 0.11294E+01 ppm1 1.704 ppm2 0.342
ASSI {15662}
  ( segid "PROT" and resid 74 and name HE% )
  ( segid "PROT" and resid 18 and name HD1% )
  3.100 2.400 2.400 peak 15662 weight 0.10000E+01 volume 0.10555E+01 ppm1 6.968 ppm2 0.519
ASSI {15672}
  ( segid "PROT" and resid 68 and name HD% )
  ( segid "PROT" and resid 18 and name HD1% )
  3.000 2.200 2.200 peak 15672 weight 0.10000E+01 volume 0.13402E+01 ppm1 7.213 ppm2 0.512
ASSI {15692}
  ( ( segid "PROT" and resid 17 and name HB ) )
  ( segid "PROT" and resid 18 and name HD2% )
  3.000 2.200 2.200 peak 15692 weight 0.10000E+01 volume 0.14210E+01 ppm1 4.288 ppm2 -0.161
ASSI {15702}

```

```

(( segid "PROT" and resid 22 and name HA ))
(( segid "PROT" and resid 22 and name HB1 ))
2.800 2.000 2.000 peak 15702 weight 0.10000E+01 volume 0.21005E+01 ppm1 4.154 ppm2 2.131
ASSI {15722}
( segid "PROT" and resid 22 and name HD1%)
(( segid "PROT" and resid 22 and name HA ))
2.700 1.800 1.800 peak 15722 weight 0.10000E+01 volume 0.23790E+01 ppm1 1.105 ppm2 4.152
ASSI {15762}
(( segid "PROT" and resid 22 and name HA ))
(( segid "PROT" and resid 22 and name HG ))
2.900 2.100 2.100 peak 15762 weight 0.10000E+01 volume 0.18179E+01 ppm1 4.155 ppm2 1.788
ASSI {15772}
(( segid "PROT" and resid 22 and name HB2 ))
( segid "PROT" and resid 22 and name HD1%)
2.300 1.300 1.300 peak 15772 weight 0.10000E+01 volume 0.71485E+01 ppm1 1.734 ppm2 1.106
ASSI {15782}
(( segid "PROT" and resid 22 and name HB2 ))
( segid "PROT" and resid 22 and name HD2%)
2.300 1.300 1.300 peak 15782 weight 0.10000E+01 volume 0.69966E+01 ppm1 1.730 ppm2 1.049
ASSI {15822}
(( segid "PROT" and resid 56 and name HA ))
(( segid "PROT" and resid 56 and name HB1 ))
3.000 2.200 2.200 peak 15822 weight 0.10000E+01 volume 0.13848E+01 ppm1 4.066 ppm2 2.092
ASSI {15832}
(( segid "PROT" and resid 56 and name HG ))
(( segid "PROT" and resid 56 and name HA ))
2.500 1.600 1.600 peak 15832 weight 0.10000E+01 volume 0.45909E+01 ppm1 1.772 ppm2 4.074
ASSI {15842}
(( segid "PROT" and resid 56 and name HG ))
(( segid "PROT" and resid 56 and name HB1 ))
2.400 1.400 1.400 peak 15842 weight 0.10000E+01 volume 0.48109E+01 ppm1 1.765 ppm2 2.115
ASSI {15852}
(( segid "PROT" and resid 56 and name HA ))
( segid "PROT" and resid 56 and name HD2%)
2.200 1.200 1.200 peak 15852 weight 0.10000E+01 volume 0.97607E+01 ppm1 4.064 ppm2 0.677
ASSI {15862}
(( segid "PROT" and resid 56 and name HB1 ))
( segid "PROT" and resid 56 and name HD2%)
2.600 1.700 1.700 peak 15862 weight 0.10000E+01 volume 0.36257E+01 ppm1 2.123 ppm2 0.678
ASSI {15872}
( segid "PROT" and resid 56 and name HD1%)
( segid "PROT" and resid 56 and name HD2%)
2.000 1.000 1.000 peak 15872 weight 0.10000E+01 volume 0.14850E+02 ppm1 0.980 ppm2 0.676
ASSI {15882}
( segid "PROT" and resid 22 and name HD2%)
( segid "PROT" and resid 56 and name HD2%)
2.000 1.000 1.000 peak 15882 weight 0.10000E+01 volume 0.15848E+02 ppm1 1.058 ppm2 0.676
ASSI {15902}
( segid "PROT" and resid 59 and name HE%)
( segid "PROT" and resid 56 and name HD2%)
3.200 2.600 2.300 peak 15902 weight 0.10000E+01 volume 0.10042E+01 ppm1 1.306 ppm2 0.675
ASSI {15912}
(( segid "PROT" and resid 25 and name HB ))
( segid "PROT" and resid 56 and name HD2%)
3.200 2.600 2.300 peak 15912 weight 0.10000E+01 volume 0.99240E+00 ppm1 2.443 ppm2 0.681
ASSI {15922}
(( segid "PROT" and resid 59 and name HG1 ))
( segid "PROT" and resid 56 and name HD2%)
3.100 2.400 2.400 peak 15922 weight 0.10000E+01 volume 0.12677E+01 ppm1 2.648 ppm2 0.680
ASSI {15932}
(( segid "PROT" and resid 34 and name HB1 ))
( segid "PROT" and resid 56 and name HD2%)
3.100 2.400 2.400 peak 15932 weight 0.10000E+01 volume 0.11626E+01 ppm1 3.513 ppm2 0.676
ASSI {15942}
(( segid "PROT" and resid 35 and name HA ))
( segid "PROT" and resid 56 and name HD2%)
3.000 2.200 2.200 peak 15942 weight 0.10000E+01 volume 0.14845E+01 ppm1 4.342 ppm2 0.676
ASSI {15952}
( segid "PROT" and resid 78 and name HD2%)
( segid "PROT" and resid 56 and name HD1%)
3.300 2.700 2.200 peak 15952 weight 0.10000E+01 volume 0.84570E+00 ppm1 0.179 ppm2 0.984
ASSI {15972}
(( segid "PROT" and resid 31 and name HA ))
( segid "PROT" and resid 56 and name HD1%)
3.200 2.600 2.300 peak 15972 weight 0.10000E+01 volume 0.10184E+01 ppm1 4.434 ppm2 0.979
ASSI {15982}
( segid "PROT" and resid 63 and name HD1%)
(( segid "PROT" and resid 63 and name HA ))
3.200 2.600 2.300 peak 15982 weight 0.10000E+01 volume 0.98600E+00 ppm1 0.919 ppm2 4.719
ASSI {15992}
(( segid "PROT" and resid 63 and name HG ))
(( segid "PROT" and resid 63 and name HA ))
3.100 2.400 2.400 peak 15992 weight 0.10000E+01 volume 0.11802E+01 ppm1 1.865 ppm2 4.719
ASSI {16002}
(( segid "PROT" and resid 63 and name HB2 ))
(( segid "PROT" and resid 63 and name HA ))
3.000 2.200 2.200 peak 16002 weight 0.10000E+01 volume 0.14688E+01 ppm1 1.972 ppm2 4.719
ASSI {16012}
(( segid "PROT" and resid 67 and name HB2 ))

```

```

(( segid "PROT" and resid 63 and name HA ))
3.400 2.900 2.100 peak 16012 weight 0.10000E+01 volume 0.71580E+00 ppm1 2.086 ppm2 4.719
ASSI {16052}
(( segid "PROT" and resid 63 and name HA ))
(( segid "PROT" and resid 63 and name HB1 ))
3.000 2.200 2.200 peak 16052 weight 0.10000E+01 volume 0.14729E+01 ppm1 4.717 ppm2 2.352
ASSI {16092}
(( segid "PROT" and resid 63 and name HG ))
(( segid "PROT" and resid 63 and name HD1% ))
2.200 1.200 1.200 peak 16092 weight 0.10000E+01 volume 0.90416E+01 ppm1 1.852 ppm2 0.922
ASSI {16102}
(( segid "PROT" and resid 63 and name HB2 ))
(( segid "PROT" and resid 63 and name HD1% ))
2.500 1.600 1.600 peak 16102 weight 0.10000E+01 volume 0.45661E+01 ppm1 1.966 ppm2 0.923
ASSI {16112}
(( segid "PROT" and resid 63 and name HB1 ))
(( segid "PROT" and resid 63 and name HD1% ))
2.400 1.400 1.400 peak 16112 weight 0.10000E+01 volume 0.51188E+01 ppm1 2.355 ppm2 0.918
ASSI {16142}
(( segid "PROT" and resid 63 and name HB2 ))
(( segid "PROT" and resid 63 and name HD2% ))
2.400 1.400 1.400 peak 16142 weight 0.10000E+01 volume 0.52687E+01 ppm1 1.965 ppm2 1.078
ASSI {16152}
(( segid "PROT" and resid 73 and name HG ))
(( segid "PROT" and resid 73 and name HA ))
2.500 1.600 1.600 peak 16152 weight 0.10000E+01 volume 0.40193E+01 ppm1 1.802 ppm2 4.260
ASSI {16182}
(( segid "PROT" and resid 68 and name HA ))
(( segid "PROT" and resid 73 and name HB1 ))
3.200 2.600 2.300 peak 16182 weight 0.10000E+01 volume 0.87100E+00 ppm1 4.581 ppm2 2.019
ASSI {16192}
(( segid "PROT" and resid 68 and name HA ))
(( segid "PROT" and resid 73 and name HB2 ))
3.200 2.600 2.300 peak 16192 weight 0.10000E+01 volume 0.87570E+00 ppm1 4.575 ppm2 1.929
ASSI {16202}
(( segid "PROT" and resid 68 and name HE% ))
(( segid "PROT" and resid 73 and name HB2 ))
3.000 2.200 2.200 peak 16202 weight 0.10000E+01 volume 0.13823E+01 ppm1 7.316 ppm2 1.918
ASSI {16232}
(( segid "PROT" and resid 68 and name HD% ))
(( segid "PROT" and resid 73 and name HB ))
3.000 2.200 2.200 peak 16232 weight 0.10000E+01 volume 0.14152E+01 ppm1 7.214 ppm2 1.805
ASSI {16262}
(( segid "PROT" and resid 68 and name HA ))
(( segid "PROT" and resid 73 and name HD2% ))
3.000 2.200 2.200 peak 16262 weight 0.10000E+01 volume 0.13485E+01 ppm1 4.573 ppm2 0.922
ASSI {16272}
(( segid "PROT" and resid 68 and name HD% ))
(( segid "PROT" and resid 73 and name HD2% ))
3.000 2.200 2.200 peak 16272 weight 0.10000E+01 volume 0.13605E+01 ppm1 7.216 ppm2 0.927
ASSI {16282}
(( segid "PROT" and resid 68 and name HE% ))
(( segid "PROT" and resid 73 and name HD2% ))
3.000 2.200 2.200 peak 16282 weight 0.10000E+01 volume 0.14572E+01 ppm1 7.317 ppm2 0.931
ASSI {16292}
(( segid "PROT" and resid 68 and name HE% ))
(( segid "PROT" and resid 73 and name HD1% ))
3.100 2.400 2.400 peak 16292 weight 0.10000E+01 volume 0.12364E+01 ppm1 7.315 ppm2 0.976
ASSI {16302}
(( segid "PROT" and resid 78 and name HG ))
(( segid "PROT" and resid 78 and name HA ))
2.600 1.700 1.700 peak 16302 weight 0.10000E+01 volume 0.36564E+01 ppm1 0.695 ppm2 3.417
ASSI {16312}
(( segid "PROT" and resid 78 and name HB2 ))
(( segid "PROT" and resid 78 and name HA ))
2.400 1.400 1.400 peak 16312 weight 0.10000E+01 volume 0.51147E+01 ppm1 0.467 ppm2 3.415
ASSI {16332}
(( segid "PROT" and resid 78 and name HB1 ))
(( segid "PROT" and resid 78 and name HD2% ))
2.300 1.300 1.300 peak 16332 weight 0.10000E+01 volume 0.63946E+01 ppm1 0.742 ppm2 0.197
ASSI {16352}
(( segid "PROT" and resid 78 and name HB2 ))
(( segid "PROT" and resid 78 and name HD1% ))
2.400 1.400 1.400 peak 16352 weight 0.10000E+01 volume 0.55770E+01 ppm1 0.476 ppm2 0.092
ASSI {16392}
(( segid "PROT" and resid 81 and name HB ))
(( segid "PROT" and resid 78 and name HD1% ))
3.200 2.600 2.300 peak 16392 weight 0.10000E+01 volume 0.10149E+01 ppm1 1.461 ppm2 0.093
ASSI {16402}
(( segid "PROT" and resid 106 and name HB2 ))
(( segid "PROT" and resid 78 and name HD1% ))
3.000 2.200 2.200 peak 16402 weight 0.10000E+01 volume 0.14513E+01 ppm1 3.146 ppm2 0.091
ASSI {16422}
(( segid "PROT" and resid 102 and name HG ))
(( segid "PROT" and resid 102 and name HB1 ))
2.600 1.700 1.700 peak 16422 weight 0.10000E+01 volume 0.30300E+01 ppm1 1.593 ppm2 1.484
ASSI {16442}
(( segid "PROT" and resid 102 and name HG ))
(( segid "PROT" and resid 102 and name HD1% ))

```

```

1.900      0.900      0.900 peak 16442 weight 0.10000E+01 volume 0.19614E+02 ppm1 1.596 ppm2 0.756
ASSI {16462}
(( segid "PROT" and resid 102 and name HA ))
( segid "PROT" and resid 102 and name HD1%)
2.700      1.800      1.800 peak 16462 weight 0.10000E+01 volume 0.28719E+01 ppm1 3.722 ppm2 0.763
ASSI {16472}
( segid "PROT" and resid 82 and name HE% )
(( segid "PROT" and resid 102 and name HB2 ))
3.300      2.700      2.200 peak 16472 weight 0.10000E+01 volume 0.74030E+00 ppm1 6.487 ppm2 1.270
ASSI {16492}
( segid "PROT" and resid 102 and name HD2%)
(( segid "PROT" and resid 102 and name HG ))
2.100      1.100      1.100 peak 16492 weight 0.10000E+01 volume 0.12673E+02 ppm1 0.763 ppm2 1.591
ASSI {16512}
(( segid "PROT" and resid 28 and name HD2 ))
( segid "PROT" and resid 102 and name HD2%)
3.000      2.200      2.200 peak 16512 weight 0.10000E+01 volume 0.14555E+01 ppm1 5.006 ppm2 0.767
ASSI {16552}
( segid "PROT" and resid 115 and name HD1%)
(( segid "PROT" and resid 115 and name HA ))
2.200      1.200      1.200 peak 16552 weight 0.10000E+01 volume 0.80718E+01 ppm1 0.763 ppm2 4.251
ASSI {16572}
(( segid "PROT" and resid 21 and name HB ))
(( segid "PROT" and resid 21 and name HA ))
2.700      1.800      1.800 peak 16572 weight 0.10000E+01 volume 0.25287E+01 ppm1 1.948 ppm2 3.798
ASSI {16582}
(( segid "PROT" and resid 21 and name HG11))
(( segid "PROT" and resid 21 and name HA ))
2.600      1.700      1.700 peak 16582 weight 0.10000E+01 volume 0.33367E+01 ppm1 1.786 ppm2 3.802
ASSI {16602}
(( segid "PROT" and resid 21 and name HG12))
(( segid "PROT" and resid 21 and name HA ))
2.500      1.600      1.600 peak 16602 weight 0.10000E+01 volume 0.46692E+01 ppm1 1.074 ppm2 3.798
ASSI {16622}
(( segid "PROT" and resid 24 and name HG2 ))
(( segid "PROT" and resid 21 and name HA ))
2.700      1.800      1.800 peak 16622 weight 0.10000E+01 volume 0.26895E+01 ppm1 2.502 ppm2 3.797
ASSI {16632}
(( segid "PROT" and resid 24 and name HB2 ))
(( segid "PROT" and resid 21 and name HA ))
3.200      2.600      2.300 peak 16632 weight 0.10000E+01 volume 0.10089E+01 ppm1 2.430 ppm2 3.797
ASSI {16642}
(( segid "PROT" and resid 21 and name HA ))
( segid "PROT" and resid 21 and name HD1%)
2.500      1.600      1.600 peak 16642 weight 0.10000E+01 volume 0.40517E+01 ppm1 3.800 ppm2 0.655
ASSI {16652}
(( segid "PROT" and resid 21 and name HG12))
(( segid "PROT" and resid 21 and name HB ))
2.600      1.700      1.700 peak 16652 weight 0.10000E+01 volume 0.33647E+01 ppm1 1.074 ppm2 1.950
ASSI {16672}
(( segid "PROT" and resid 21 and name HB ))
( segid "PROT" and resid 21 and name HG2%)
2.000      1.000      1.000 peak 16672 weight 0.10000E+01 volume 0.16452E+02 ppm1 1.947 ppm2 1.019
ASSI {16682}
( segid "PROT" and resid 18 and name HD2%)
(( segid "PROT" and resid 21 and name HB ))
3.300      2.700      2.200 peak 16682 weight 0.10000E+01 volume 0.83910E+00 ppm1 -0.157 ppm2 1.947
ASSI {16692}
(( segid "PROT" and resid 109 and name HD1 ))
(( segid "PROT" and resid 21 and name HG12))
3.100      2.400      2.400 peak 16692 weight 0.10000E+01 volume 0.12669E+01 ppm1 1.416 ppm2 1.077
ASSI {16702}
( segid "PROT" and resid 106 and name HD% )
(( segid "PROT" and resid 21 and name HG11))
3.300      2.700      2.200 peak 16702 weight 0.10000E+01 volume 0.73640E+00 ppm1 6.962 ppm2 1.781
ASSI {16712}
(( segid "PROT" and resid 21 and name HG12))
( segid "PROT" and resid 21 and name HD1%)
2.100      1.100      1.100 peak 16712 weight 0.10000E+01 volume 0.12596E+02 ppm1 1.078 ppm2 0.650
ASSI {16722}
( segid "PROT" and resid 18 and name HD2%)
( segid "PROT" and resid 21 and name HG2%)
3.000      2.200      2.200 peak 16722 weight 0.10000E+01 volume 0.13840E+01 ppm1 -0.159 ppm2 1.020
ASSI {16742}
(( segid "PROT" and resid 17 and name HA ))
( segid "PROT" and resid 21 and name HD1%)
3.100      2.400      2.400 peak 16742 weight 0.10000E+01 volume 0.11559E+01 ppm1 3.975 ppm2 0.660
ASSI {16782}
(( segid "PROT" and resid 47 and name HA ))
(( segid "PROT" and resid 50 and name HB ))
3.200      2.600      2.300 peak 16782 weight 0.10000E+01 volume 0.98740E+00 ppm1 4.139 ppm2 1.249
ASSI {16792}
(( segid "PROT" and resid 50 and name HB ))
(( segid "PROT" and resid 50 and name HA ))
2.600      1.700      1.700 peak 16792 weight 0.10000E+01 volume 0.33271E+01 ppm1 1.252 ppm2 3.951
ASSI {16822}
(( segid "PROT" and resid 50 and name HA ))
(( segid "PROT" and resid 50 and name HG12))
3.000      2.200      2.200 peak 16822 weight 0.10000E+01 volume 0.14239E+01 ppm1 3.956 ppm2 0.190

```

```

ASSI {16832}
(( segid "PROT" and resid 53 and name HG2 ))
(( segid "PROT" and resid 50 and name HB ))
3.300 2.700 2.200 peak 16832 weight 0.10000E+01 volume 0.81300E+00 ppm1 1 933 ppm2 1.256
ASSI {16842}
(( segid "PROT" and resid 50 and name HB ))
(( segid "PROT" and resid 50 and name HG11))
2.600 1.700 1.700 peak 16842 weight 0.10000E+01 volume 0.29784E+01 ppm1 1.250 ppm2 0.830
ASSI {16882}
(( segid "PROT" and resid 49 and name HB ))
(( segid "PROT" and resid 50 and name HG12))
3.300 2.700 2.200 peak 16882 weight 0.10000E+01 volume 0.76190E+00 ppm1 1.928 ppm2 0.182
ASSI {16892}
(( segid "PROT" and resid 49 and name HB ))
(( segid "PROT" and resid 50 and name HD1%))
3.100 2.400 2.400 peak 16892 weight 0.10000E+01 volume 0.12022E+01 ppm1 1.926 ppm2 0.586
ASSI {16902}
(( segid "PROT" and resid 87 and name HG1 ))
(( segid "PROT" and resid 50 and name HD1%))
3.200 2.600 2.300 peak 16902 weight 0.10000E+01 volume 0.92330E+00 ppm1 2.438 ppm2 0.586
ASSI {16912}
(( segid "PROT" and resid 85 and name HN ))
(( segid "PROT" and resid 50 and name HD1%))
3.200 2.600 2.300 peak 16912 weight 0.10000E+01 volume 0.98650E+00 ppm1 6.889 ppm2 0.579
ASSI {16952}
(( segid "PROT" and resid 53 and name HD1 ))
(( segid "PROT" and resid 50 and name HG2%))
3.200 2.600 2.300 peak 16952 weight 0.10000E+01 volume 0.98080E+00 ppm1 3.648 ppm2 0.420
ASSI {16982}
(( segid "PROT" and resid 104 and name HD1 ))
(( segid "PROT" and resid 101 and name HA ))
3.100 2.400 2.400 peak 16982 weight 0.10000E+01 volume 0.10838E+01 ppm1 1.729 ppm2 3.693
ASSI {16992}
(( segid "PROT" and resid 101 and name HB ))
(( segid "PROT" and resid 101 and name HG12))
2.400 1.400 1.400 peak 16992 weight 0.10000E+01 volume 0.51879E+01 ppm1 1.948 ppm2 1.241
ASSI {17012}
(( segid "PROT" and resid 101 and name HB ))
(( segid "PROT" and resid 101 and name HD1%))
2.100 1.100 1.100 peak 17012 weight 0.10000E+01 volume 0.11433E+02 ppm1 1.949 ppm2 0.993
ASSI {17022}
(( segid "PROT" and resid 101 and name HB ))
(( segid "PROT" and resid 101 and name HG2%))
1.900 0.900 0.900 peak 17022 weight 0.10000E+01 volume 0.20229E+02 ppm1 1.949 ppm2 1.032
ASSI {17032}
(( segid "PROT" and resid 101 and name HG11))
(( segid "PROT" and resid 101 and name HG2%))
2.100 1.100 1.100 peak 17032 weight 0.10000E+01 volume 0.10554E+02 ppm1 1.899 ppm2 1.032
ASSI {17042}
(( segid "PROT" and resid 30 and name HB1 ))
(( segid "PROT" and resid 101 and name HB ))
3.200 2.600 2.300 peak 17042 weight 0.10000E+01 volume 0.89790E+00 ppm1 4.360 ppm2 1.943
ASSI {17082}
(( segid "PROT" and resid 101 and name HG12))
(( segid "PROT" and resid 101 and name HG2%))
2.100 1.100 1.100 peak 17082 weight 0.10000E+01 volume 0.11790E+02 ppm1 1.241 ppm2 1.032
ASSI {17122}
(( segid "PROT" and resid 30 and name HB1 ))
(( segid "PROT" and resid 101 and name HD1%))
3.000 2.200 2.200 peak 17122 weight 0.10000E+01 volume 0.13541E+01 ppm1 4.342 ppm2 0.990
ASSI {17152}
(( segid "PROT" and resid 110 and name HA ))
(( segid "PROT" and resid 110 and name HG12))
2.400 1.400 1.400 peak 17152 weight 0.10000E+01 volume 0.54547E+01 ppm1 3.863 ppm2 1.098
ASSI {17162}
(( segid "PROT" and resid 110 and name HB ))
(( segid "PROT" and resid 110 and name HD1%))
2.300 1.300 1.300 peak 17162 weight 0.10000E+01 volume 0.78140E+01 ppm1 1.798 ppm2 0.575
ASSI {17192}
(( segid "PROT" and resid 110 and name HG2%))
(( segid "PROT" and resid 110 and name HD1%))
1.900 0.900 0.900 peak 17192 weight 0.10000E+01 volume 0.19792E+02 ppm1 0.694 ppm2 0.568
ASSI {17232}
(( segid "PROT" and resid 75 and name HB2 ))
(( segid "PROT" and resid 110 and name HD1%))
3.100 2.400 2.400 peak 17232 weight 0.10000E+01 volume 0.11996E+01 ppm1 2.651 ppm2 0.571
ASSI {17282}
(( segid "PROT" and resid 116 and name HD1%))
(( segid "PROT" and resid 116 and name HB ))
2.100 1.100 1.100 peak 17282 weight 0.10000E+01 volume 0.10804E+02 ppm1 0.832 ppm2 1.851
ASSI {17292}
(( segid "PROT" and resid 110 and name HD1%))
(( segid "PROT" and resid 116 and name HB ))
3.200 2.600 2.300 peak 17292 weight 0.10000E+01 volume 0.95100E+00 ppm1 0.564 ppm2 1.846
ASSI {17312}
(( segid "PROT" and resid 9 and name HA ))
(( segid "PROT" and resid 9 and name HB2 ))
2.400 1.400 1.400 peak 17312 weight 0.10000E+01 volume 0.58458E+01 ppm1 4.363 ppm2 1.828
ASSI {17322}

```



```

(( segid "PROT" and resid 9      and name HD1 ))
(( segid "PROT" and resid 9      and name HB2 ))
2.500    1.600    1.600 peak 17322 weight 0.10000E+01 volume 0.39205E+01 ppm1 3.223 ppm2 1.831
ASSI {17332}
(( segid "PROT" and resid 9      and name HB1 ))
(( segid "PROT" and resid 9      and name HD1 ))
2.300    1.300    1.300 peak 17332 weight 0.10000E+01 volume 0.77754E+01 ppm1 1.879 ppm2 3.221
ASSI {17362}
(( segid "PROT" and resid 51     and name HG1 ))
(( segid "PROT" and resid 51     and name HA ))
2.500    1.600    1.600 peak 17362 weight 0.10000E+01 volume 0.39373E+01 ppm1 1.354 ppm2 3.879
ASSI {17372}
(( segid "PROT" and resid 51     and name HB1 ))
(( segid "PROT" and resid 51     and name HA ))
2.400    1.400    1.400 peak 17372 weight 0.10000E+01 volume 0.53335E+01 ppm1 1.390 ppm2 3.877
ASSI {17382}
(( segid "PROT" and resid 51     and name HB1 ))
(( segid "PROT" and resid 51     and name HD1 ))
2.300    1.300    1.300 peak 17382 weight 0.10000E+01 volume 0.65385E+01 ppm1 1.382 ppm2 3.022
ASSI {17402}
(( segid "PROT" and resid 51     and name HA ))
(( segid "PROT" and resid 51     and name HG2 ))
2.300    1.300    1.300 peak 17402 weight 0.10000E+01 volume 0.65716E+01 ppm1 3.878 ppm2 1.196
ASSI {17442}
(( segid "PROT" and resid 51     and name HG2 ))
(( segid "PROT" and resid 51     and name HB1 ))
1.900    0.900    0.900 peak 17442 weight 0.10000E+01 volume 0.20102E+02 ppm1 1.197 ppm2 1.381
ASSI {17452}
(( segid "PROT" and resid 51     and name HG2 ))
(( segid "PROT" and resid 51     and name HG1 ))
2.000    1.000    1.000 peak 17452 weight 0.10000E+01 volume 0.17189E+02 ppm1 1.196 ppm2 1.350
ASSI {17472}
(( segid "PROT" and resid 110    and name HG2% ))
(( segid "PROT" and resid 116    and name HG11 ))
3.000    2.200    2.200 peak 17472 weight 0.10000E+01 volume 0.13662E+01 ppm1 0.683 ppm2 1.349
ASSI {17482}
(( segid "PROT" and resid 110    and name HD1% ))
(( segid "PROT" and resid 116    and name HG11 ))
3.100    2.400    2.400 peak 17482 weight 0.10000E+01 volume 0.10860E+01 ppm1 0.568 ppm2 1.350
ASSI {17502}
(( segid "PROT" and resid 66     and name HB2 ))
(( segid "PROT" and resid 66     and name HA ))
2.300    1.300    1.300 peak 17502 weight 0.10000E+01 volume 0.62411E+01 ppm1 2.051 ppm2 4.445
ASSI {17512}
(( segid "PROT" and resid 66     and name HA ))
(( segid "PROT" and resid 66     and name HG2 ))
2.500    1.600    1.600 peak 17512 weight 0.10000E+01 volume 0.37845E+01 ppm1 4.442 ppm2 1.564
ASSI {17532}
(( segid "PROT" and resid 66     and name HA ))
(( segid "PROT" and resid 66     and name HD2 ))
2.300    2.300    2.200 peak 17532 weight 0.10000E+01 volume 0.71490E+01 ppm1 4.443 ppm2 3.061
ASSI {17542}
(( segid "PROT" and resid 66     and name HD1 ))
(( segid "PROT" and resid 66     and name HB2 ))
3.100    2.400    2.400 peak 17542 weight 0.10000E+01 volume 0.12368E+01 ppm1 3.103 ppm2 2.051
ASSI {17552}
(( segid "PROT" and resid 66     and name HD2 ))
(( segid "PROT" and resid 66     and name HB1 ))
3.000    2.200    2.200 peak 17552 weight 0.10000E+01 volume 0.12950E+01 ppm1 3.068 ppm2 2.124
ASSI {17562}
(( segid "PROT" and resid 66     and name HD1 ))
(( segid "PROT" and resid 66     and name HB1 ))
3.100    2.400    2.400 peak 17562 weight 0.10000E+01 volume 0.12382E+01 ppm1 3.103 ppm2 2.124
ASSI {17572}
(( segid "PROT" and resid 66     and name HD1 ))
(( segid "PROT" and resid 66     and name HG2 ))
2.500    1.600    1.600 peak 17572 weight 0.10000E+01 volume 0.38907E+01 ppm1 3.103 ppm2 1.564
ASSI {17582}
(( segid "PROT" and resid 66     and name HD2 ))
(( segid "PROT" and resid 66     and name HG1 ))
2.500    1.600    1.600 peak 17582 weight 0.10000E+01 volume 0.40198E+01 ppm1 3.063 ppm2 1.614
ASSI {17592}
(( segid "PROT" and resid 66     and name HD2 ))
(( segid "PROT" and resid 66     and name HG2 ))
2.600    1.700    1.700 peak 17592 weight 0.10000E+01 volume 0.35354E+01 ppm1 3.065 ppm2 1.564
ASSI {17612}
(( segid "PROT" and resid 80     and name HD2 ))
(( segid "PROT" and resid 80     and name HB2 ))
3.000    2.200    2.200 peak 17612 weight 0.10000E+01 volume 0.14931E+01 ppm1 3.325 ppm2 1.958
ASSI {17632}
(( segid "PROT" and resid 80     and name HB2 ))
(( segid "PROT" and resid 80     and name HA ))
2.400    1.400    1.400 peak 17632 weight 0.10000E+01 volume 0.57680E+01 ppm1 1.956 ppm2 4.098
ASSI {17652}
(( segid "PROT" and resid 80     and name HG1 ))
(( segid "PROT" and resid 80     and name HA ))
2.300    1.300    1.300 peak 17652 weight 0.10000E+01 volume 0.72244E+01 ppm1 1.783 ppm2 4.098
ASSI {17672}
(( segid "PROT" and resid 19     and name HB2 ))

```

```

(( segid "PROT" and resid 19 and name HA ))
2.500 1.600 1.600 peak 17672 weight 0.10000E+01 volume 0.39072E+01 ppm1 1.408 ppm2 3.718
ASSI {17692}
(( segid "PROT" and resid 19 and name HA ))
(( segid "PROT" and resid 19 and name HD1 ))
2.900 2.100 2.100 peak 17692 weight 0.10000E+01 volume 0.16489E+01 ppm1 3.722 ppm2 1.622
ASSI {17712}
(( segid "PROT" and resid 22 and name HB1 ))
(( segid "PROT" and resid 19 and name HA ))
2.900 2.100 2.100 peak 17712 weight 0.10000E+01 volume 0.18959E+01 ppm1 2.124 ppm2 3.718
ASSI {17752}
(( segid "PROT" and resid 109 and name HE1 ))
(( segid "PROT" and resid 109 and name HA ))
3.300 2.700 2.200 peak 17752 weight 0.10000E+01 volume 0.80270E+00 ppm1 2.619 ppm2 4.069
ASSI {17772}
(( segid "PROT" and resid 109 and name HA ))
(( segid "PROT" and resid 109 and name HB1 ))
2.400 1.400 1.400 peak 17772 weight 0.10000E+01 volume 0.47284E+01 ppm1 4.070 ppm2 1.762
ASSI {17802}
(( segid "PROT" and resid 109 and name HD1 ))
(( segid "PROT" and resid 109 and name HB1 ))
2.400 1.400 1.400 peak 17802 weight 0.10000E+01 volume 0.55212E+01 ppm1 1.415 ppm2 1.770
ASSI {17812}
(( segid "PROT" and resid 109 and name HD1 ))
(( segid "PROT" and resid 109 and name HB2 ))
2.700 1.800 1.800 peak 17812 weight 0.10000E+01 volume 0.25524E+01 ppm1 1.415 ppm2 1.587
ASSI {17822}
(( segid "PROT" and resid 21 and name HD1* ))
(( segid "PROT" and resid 109 and name HB1 ))
3.300 2.700 2.200 peak 17822 weight 0.10000E+01 volume 0.75320E+00 ppm1 0.658 ppm2 1.765
ASSI {17842}
(( segid "PROT" and resid 21 and name HG2* ))
(( segid "PROT" and resid 109 and name HB1 ))
3.200 2.600 2.300 peak 17842 weight 0.10000E+01 volume 0.10322E+01 ppm1 1.023 ppm2 1.765
ASSI {17862}
(( segid "PROT" and resid 109 and name HB1 ))
(( segid "PROT" and resid 109 and name HB2 ))
2.200 1.200 1.200 peak 17862 weight 0.10000E+01 volume 0.97810E+01 ppm1 1.762 ppm2 1.587
ASSI {17872}
(( segid "PROT" and resid 111 and name HA ))
(( segid "PROT" and resid 111 and name HB1 ))
2.600 1.700 1.700 peak 17872 weight 0.10000E+01 volume 0.29552E+01 ppm1 4.081 ppm2 2.942
ASSI {17882}
(( segid "PROT" and resid 111 and name HG2 ))
(( segid "PROT" and resid 111 and name HA ))
2.600 1.700 1.700 peak 17882 weight 0.10000E+01 volume 0.34200E+01 ppm1 1.348 ppm2 4.085
ASSI {17892}
(( segid "PROT" and resid 111 and name HG1 ))
(( segid "PROT" and resid 111 and name HA ))
2.500 1.600 1.600 peak 17892 weight 0.10000E+01 volume 0.42726E+01 ppm1 1.450 ppm2 4.085
ASSI {17902}
(( segid "PROT" and resid 111 and name HB2 ))
(( segid "PROT" and resid 111 and name HA ))
2.100 1.100 1.100 peak 17902 weight 0.10000E+01 volume 0.12554E+02 ppm1 1.791 ppm2 4.077
ASSI {17912}
(( segid "PROT" and resid 111 and name HB1 ))
(( segid "PROT" and resid 111 and name HB2 ))
3.300 2.700 2.200 peak 17912 weight 0.10000E+01 volume 0.85920E+00 ppm1 2.954 ppm2 1.785
ASSI {17922}
(( segid "PROT" and resid 111 and name HG2 ))
(( segid "PROT" and resid 111 and name HB2 ))
2.300 1.300 1.300 peak 17922 weight 0.10000E+01 volume 0.63823E+01 ppm1 1.349 ppm2 1.793
ASSI {17932}
(( segid "PROT" and resid 111 and name HG1 ))
(( segid "PROT" and resid 111 and name HB1 ))
2.200 1.200 1.200 peak 17932 weight 0.10000E+01 volume 0.87727E+01 ppm1 1.451 ppm2 1.913
ASSI {17962}
(( segid "PROT" and resid 111 and name HD1 ))
(( segid "PROT" and resid 111 and name HG1 ))
1.700 0.700 0.700 peak 17962 weight 0.10000E+01 volume 0.37190E+02 ppm1 1.643 ppm2 1.450
ASSI {17972}
(( segid "PROT" and resid 8 and name HA ))
(( segid "PROT" and resid 8 and name HB2 ))
2.500 1.600 1.600 peak 17972 weight 0.10000E+01 volume 0.37603E+01 ppm1 4.463 ppm2 1.917
ASSI {17992}
(( segid "PROT" and resid 8 and name HA ))
(( segid "PROT" and resid 8 and name HD2 ))
3.300 2.700 2.200 peak 17992 weight 0.10000E+01 volume 0.82050E+00 ppm1 4.463 ppm2 3.708
ASSI {18002}
(( segid "PROT" and resid 8 and name HD1 ))
(( segid "PROT" and resid 8 and name HA ))
3.000 2.200 2.200 peak 18002 weight 0.10000E+01 volume 0.14398E+01 ppm1 3.873 ppm2 4.445
ASSI {18102}
(( segid "PROT" and resid 37 and name HA ))
(( segid "PROT" and resid 37 and name HG2 ))
2.700 1.800 1.800 peak 18102 weight 0.10000E+01 volume 0.24227E+01 ppm1 4.277 ppm2 2.039
ASSI {18112}
(( segid "PROT" and resid 37 and name HA ))
(( segid "PROT" and resid 37 and name HD1 ))

```

3.000	2.200	2.200	peak 18112	weight	0.10000E+01	volume	0.13649E+01	ppm1	4.276	ppm2	3.706
ASSI {18122}											
((segid "PROT" and resid 37			and name HG2))								
((segid "PROT" and resid 37			and name HB1))								
1.900	0.900	0.900	peak 18122	weight	0.10000E+01	volume	0.24810E+02	ppm1	2.042	ppm2	2.389
ASSI {18142}											
((segid "PROT" and resid 37			and name HD1))								
((segid "PROT" and resid 37			and name HG2))								
2.200	1.200	1.200	peak 18142	weight	0.10000E+01	volume	0.94260E+01	ppm1	3.715	ppm2	2.040
ASSI {18192}											
((segid "PROT" and resid 44			and name HB1))								
((segid "PROT" and resid 44			and name HD2))								
3.000	2.200	2.200	peak 18192	weight	0.10000E+01	volume	0.14606E+01	ppm1	2.413	ppm2	3.573
ASSI {18202}											
((segid "PROT" and resid 44			and name HB1))								
((segid "PROT" and resid 44			and name HD1))								
3.000	2.200	2.200	peak 18202	weight	0.10000E+01	volume	0.14741E+01	ppm1	2.413	ppm2	3.838
ASSI {18222}											
((segid "PROT" and resid 44			and name HB2))								
((segid "PROT" and resid 44			and name HB1))								
1.900	0.900	0.900	peak 18222	weight	0.10000E+01	volume	0.21799E+02	ppm1	2.062	ppm2	2.415
ASSI {18262}											
((segid "PROT" and resid 44			and name HA))								
((segid "PROT" and resid 44			and name HD2))								
3.200	2.600	2.300	peak 18262	weight	0.10000E+01	volume	0.98750E+00	ppm1	4.553	ppm2	3.564
ASSI {18272}											
((segid "PROT" and resid 44			and name HG1))								
((segid "PROT" and resid 44			and name HB2))								
2.100	1.100	1.100	peak 18272	weight	0.10000E+01	volume	0.11240E+02	ppm1	2.207	ppm2	2.053
ASSI {18312}											
((segid "PROT" and resid 49			and name HG1%))								
((segid "PROT" and resid 49			and name HA))								
2.300	1.300	1.300	peak 18312	weight	0.10000E+01	volume	0.68598E+01	ppm1	0.962	ppm2	4.110
ASSI {18332}											
((segid "PROT" and resid 54			and name HB2))								
((segid "PROT" and resid 54			and name HA))								
3.000	2.200	2.200	peak 18332	weight	0.10000E+01	volume	0.14619E+01	ppm1	1.394	ppm2	4.986
ASSI {18352}											
((segid "PROT" and resid 54			and name HG1))								
((segid "PROT" and resid 54			and name HA))								
3.200	2.600	2.300	peak 18352	weight	0.10000E+01	volume	0.89060E+00	ppm1	2.737	ppm2	4.985
ASSI {18362}											
((segid "PROT" and resid 53			and name HA))								
((segid "PROT" and resid 54			and name HA))								
3.300	2.700	2.200	peak 18362	weight	0.10000E+01	volume	0.74720E+00	ppm1	4.121	ppm2	4.989
ASSI {18372}											
((segid "PROT" and resid 28			and name HD2))								
((segid "PROT" and resid 28			and name HB1))								
3.400	2.900	2.100	peak 18372	weight	0.10000E+01	volume	0.70920E+00	ppm1	5.011	ppm2	3.024
ASSI {18382}											
((segid "PROT" and resid 28			and name HD2))								
((segid "PROT" and resid 28			and name HB2))								
3.200	2.600	2.300	peak 18382	weight	0.10000E+01	volume	0.10243E+01	ppm1	5.011	ppm2	2.811
ASSI {18422}											
((segid "PROT" and resid 58			and name HB))								
((segid "PROT" and resid 54			and name HE%))								
3.000	2.200	2.200	peak 18422	weight	0.10000E+01	volume	0.14720E+01	ppm1	4.119	ppm2	2.005
ASSI {18452}											
((segid "PROT" and resid 54			and name HB1))								
((segid "PROT" and resid 54			and name HA))								
2.600	1.700	1.700	peak 18452	weight	0.10000E+01	volume	0.32741E+01	ppm1	2.049	ppm2	4.986
ASSI {18502}											
((segid "PROT" and resid 59			and name HB1))								
((segid "PROT" and resid 59			and name HA))								
2.700	1.800	1.800	peak 18502	weight	0.10000E+01	volume	0.24749E+01	ppm1	2.151	ppm2	4.333
ASSI {18522}											
((segid "PROT" and resid 59			and name HG2))								
((segid "PROT" and resid 59			and name HA))								
2.900	2.100	2.100	peak 18522	weight	0.10000E+01	volume	0.17299E+01	ppm1	2.558	ppm2	4.341
ASSI {18552}											
((segid "PROT" and resid 59			and name HG1))								
((segid "PROT" and resid 59			and name HE%))								
2.500	1.600	1.600	peak 18552	weight	0.10000E+01	volume	0.43371E+01	ppm1	2.651	ppm2	1.309
ASSI {18562}											
((segid "PROT" and resid 25			and name HG2%))								
((segid "PROT" and resid 59			and name HE%))								
2.600	1.700	1.700	peak 18562	weight	0.10000E+01	volume	0.30262E+01	ppm1	1.109	ppm2	1.316
ASSI {18572}											
((segid "PROT" and resid 72			and name HA))								
((segid "PROT" and resid 75			and name HB1))								
3.100	2.400	2.400	peak 18572	weight	0.10000E+01	volume	0.11453E+01	ppm1	4.083	ppm2	2.967
ASSI {18582}											
((segid "PROT" and resid 72			and name HA))								
((segid "PROT" and resid 75			and name HB2))								
3.000	2.200	2.200	peak 18582	weight	0.10000E+01	volume	0.15018E+01	ppm1	4.085	ppm2	2.640
ASSI {18592}											
((segid "PROT" and resid 75			and name HA))								
((segid "PROT" and resid 75			and name HG1))								
2.600	1.700	1.700	peak 18592	weight	0.10000E+01	volume	0.33006E+01	ppm1	4.096	ppm2	2.362

```

ASSI {18602}
(( segid "PROT" and resid 75 and name HA ))
(( segid "PROT" and resid 75 and name HG2 ))
2.300 1.300 1.300 peak 18602 weight 0.10000E+01 volume 0.65760E+01 ppm1 4.096 ppm2 2.244
ASSI {18612}
(( segid "PROT" and resid 75 and name HE% ))
(( segid "PROT" and resid 75 and name HA ))
2.000 1.000 1.000 peak 18612 weight 0.10000E+01 volume 0.14267E+02 ppm1 2.099 ppm2 4.091
ASSI {18622}
(( segid "PROT" and resid 116 and name HA ))
(( segid "PROT" and resid 75 and name HE% ))
3.200 2.600 2.300 peak 18622 weight 0.10000E+01 volume 0.10323E+01 ppm1 4.275 ppm2 2.094
ASSI {18642}
(( segid "PROT" and resid 75 and name HG2 ))
(( segid "PROT" and resid 75 and name HB1 ))
2.400 1.400 1.400 peak 18642 weight 0.10000E+01 volume 0.55414E+01 ppm1 2.240 ppm2 2.959
ASSI {18652}
(( segid "PROT" and resid 75 and name HG2 ))
(( segid "PROT" and resid 75 and name HB2 ))
2.600 1.700 1.700 peak 18652 weight 0.10000E+01 volume 0.34575E+01 ppm1 2.240 ppm2 2.640
ASSI {18662}
(( segid "PROT" and resid 75 and name HG1 ))
(( segid "PROT" and resid 75 and name HB2 ))
2.600 1.700 1.700 peak 18662 weight 0.10000E+01 volume 0.33311E+01 ppm1 2.358 ppm2 2.640
ASSI {18672}
(( segid "PROT" and resid 75 and name HG1 ))
(( segid "PROT" and resid 75 and name HB1 ))
2.600 1.700 1.700 peak 18672 weight 0.10000E+01 volume 0.33310E+01 ppm1 2.358 ppm2 2.959
ASSI {18692}
(( segid "PROT" and resid 53 and name HD2 ))
(( segid "PROT" and resid 53 and name HB1 ))
3.000 2.200 2.200 peak 18692 weight 0.10000E+01 volume 0.14740E+01 ppm1 3.443 ppm2 2.248
ASSI {18722}
(( segid "PROT" and resid 35 and name HB1 ))
(( segid "PROT" and resid 35 and name HG1 ))
2.400 1.400 1.400 peak 18722 weight 0.10000E+01 volume 0.47598E+01 ppm1 2.316 ppm2 2.903
ASSI {18732}
(( segid "PROT" and resid 35 and name HB2 ))
(( segid "PROT" and resid 35 and name HG1 ))
2.200 1.200 1.200 peak 18732 weight 0.10000E+01 volume 0.97482E+01 ppm1 2.223 ppm2 2.902
ASSI {18742}
(( segid "PROT" and resid 35 and name HG1 ))
(( segid "PROT" and resid 35 and name HA ))
2.700 1.800 1.800 peak 18742 weight 0.10000E+01 volume 0.25097E+01 ppm1 2.900 ppm2 4.342
ASSI {18752}
(( segid "PROT" and resid 35 and name HB1 ))
(( segid "PROT" and resid 35 and name HA ))
2.800 2.000 2.000 peak 18752 weight 0.10000E+01 volume 0.23049E+01 ppm1 2.320 ppm2 4.342
ASSI {18762}
(( segid "PROT" and resid 35 and name HB2 ))
(( segid "PROT" and resid 35 and name HA ))
2.400 1.400 1.400 peak 18762 weight 0.10000E+01 volume 0.56264E+01 ppm1 2.228 ppm2 4.342
ASSI {18792}
(( segid "PROT" and resid 111 and name HD1 ))
(( segid "PROT" and resid 108 and name HA ))
3.200 2.600 2.300 peak 18792 weight 0.10000E+01 volume 0.87530E+00 ppm1 1.657 ppm2 4.236
ASSI {18802}
(( segid "PROT" and resid 95 and name HB2 ))
(( segid "PROT" and resid 95 and name HA ))
3.000 2.200 2.200 peak 18802 weight 0.10000E+01 volume 0.14977E+01 ppm1 2.643 ppm2 3.648
ASSI {18812}
(( segid "PROT" and resid 33 and name HG1 ))
(( segid "PROT" and resid 95 and name HA ))
3.300 2.700 2.200 peak 18812 weight 0.10000E+01 volume 0.73410E+00 ppm1 0.269 ppm2 3.651
ASSI {18822}
(( segid "PROT" and resid 33 and name HG2 ))
(( segid "PROT" and resid 95 and name HA ))
3.400 2.900 2.100 peak 18822 weight 0.10000E+01 volume 0.67160E+00 ppm1 -0.875 ppm2 3.643
ASSI {18832}
(( segid "PROT" and resid 57 and name HD1 ))
(( segid "PROT" and resid 57 and name HA ))
2.600 1.700 1.700 peak 18832 weight 0.10000E+01 volume 0.37031E+01 ppm1 1.759 ppm2 3.910
ASSI {18842}
(( segid "PROT" and resid 106 and name HB1 ))
(( segid "PROT" and resid 103 and name HA ))
2.600 1.700 1.700 peak 18842 weight 0.10000E+01 volume 0.29665E+01 ppm1 3.358 ppm2 3.217
ASSI {18912}
(( segid "PROT" and resid 79 and name HB1 ))
(( segid "PROT" and resid 76 and name HA ))
2.700 1.800 1.800 peak 18912 weight 0.10000E+01 volume 0.26684E+01 ppm1 2.212 ppm2 4.115
ASSI {18932}
(( segid "PROT" and resid 10 and name HB1 ))
(( segid "PROT" and resid 11 and name HD1 ))
2.800 2.000 2.000 peak 18932 weight 0.10000E+01 volume 0.20083E+01 ppm1 2.788 ppm2 3.901
ASSI {18942}
(( segid "PROT" and resid 89 and name HB1 ))
(( segid "PROT" and resid 80 and name HD2 ))
3.100 2.400 2.400 peak 18942 weight 0.10000E+01 volume 0.12160E+01 ppm1 3.110 ppm2 3.947
ASSI {18952}

```

```

(( segid "PROT" and resid 89 and name HB1 ))
(( segid "PROT" and resid 90 and name HD1 ))
3.300 2.700 2.200 peak 18952 weight 0.10000E+01 volume 0.77340E+00 ppm1 3.120 ppm2 4.108
ASSI {18962}
(( segid "PROT" and resid 89 and name HB2 ))
(( segid "PROT" and resid 90 and name HD2 ))
3.200 2.600 2.300 peak 18962 weight 0.10000E+01 volume 0.10193E+01 ppm1 2.915 ppm2 3.947
ASSI {19002}
(( segid "PROT" and resid 33 and name HB2 ))
(( segid "PROT" and resid 33 and name HD2 ))
3.400 2.900 2.100 peak 19002 weight 0.10000E+01 volume 0.69650E+00 ppm1 -0.441 ppm2 1.567
ASSI {19022}
(( segid "PROT" and resid 33 and name HG1 ))
(( segid "PROT" and resid 33 and name HD1 ))
3.000 2.200 2.200 peak 19022 weight 0.10000E+01 volume 0.13980E+01 ppm1 0.280 ppm2 2.263
ASSI {19032}
(( segid "PROT" and resid 33 and name HB2 ))
(( segid "PROT" and resid 33 and name HD1 ))
3.400 2.900 2.100 peak 19032 weight 0.10000E+01 volume 0.62420E+00 ppm1 -0.431 ppm2 2.263
ASSI {19152}
(( segid "PROT" and resid 37 and name HD1 ))
(( segid "PROT" and resid 36 and name HB2 ))
2.600 1.700 1.700 peak 19152 weight 0.10000E+01 volume 0.34164E+01 ppm1 3.706 ppm2 1.800
ASSI {19202}
(( segid "PROT" and resid 33 and name HG2 ))
(( segid "PROT" and resid 33 and name HB2 ))
3.300 2.700 2.200 peak 19202 weight 0.10000E+01 volume 0.79620E+00 ppm1 -0.870 ppm2 -0.431
ASSI {19222}
(( segid "PROT" and resid 33 and name HG1 ))
(( segid "PROT" and resid 33 and name HB2 ))
3.300 2.700 2.200 peak 19222 weight 0.10000E+01 volume 0.76140E+00 ppm1 0.272 ppm2 -0.431
ASSI {19252}
(( segid "PROT" and resid 57 and name HB2 ))
(( segid "PROT" and resid 57 and name HD2 ))
2.900 2.100 2.100 peak 19252 weight 0.10000E+01 volume 0.18111E+01 ppm1 1.108 ppm2 0.913
ASSI {19322}
(( segid "PROT" and resid 15 and name HA ))
(( segid "PROT" and resid 63 and name HD2% ))
2.600 1.700 1.700 peak 19322 weight 0.10000E+01 volume 0.33620E+01 ppm1 4.057 ppm2 1.079
ASSI {19332}
(( segid "PROT" and resid 68 and name HB1 ))
(( segid "PROT" and resid 63 and name HD2% ))
2.800 2.000 2.000 peak 19332 weight 0.10000E+01 volume 0.20548E+01 ppm1 3.103 ppm2 1.080
ASSI {19342}
(( segid "PROT" and resid 33 and name HD1 ))
(( segid "PROT" and resid 33 and name HG2 ))
3.000 2.200 2.200 peak 19342 weight 0.10000E+01 volume 0.12899E+01 ppm1 2.273 ppm2 -0.868
ASSI {19372}
(( segid "PROT" and resid 34 and name HA ))
(( segid "PROT" and resid 81 and name HG2% ))
2.800 2.000 2.000 peak 19372 weight 0.10000E+01 volume 0.22956E+01 ppm1 5.007 ppm2 0.153
ASSI {19382}
(( segid "PROT" and resid 46 and name HA ))
(( segid "PROT" and resid 49 and name HG1% ))
2.500 1.600 1.600 peak 19382 weight 0.10000E+01 volume 0.38294E+01 ppm1 3.506 ppm2 0.971
ASSI {19412}
(( segid "PROT" and resid 42 and name HB2 ))
(( segid "PROT" and resid 43 and name HB% ))
3.000 2.200 2.200 peak 19412 weight 0.10000E+01 volume 0.14358E+01 ppm1 2.081 ppm2 0.973
ASSI {19422}
(( segid "PROT" and resid 82 and name HB1 ))
(( segid "PROT" and resid 99 and name HB% ))
2.400 1.400 1.400 peak 19422 weight 0.10000E+01 volume 0.49197E+01 ppm1 3.136 ppm2 1.659
ASSI {19442}
(( segid "PROT" and resid 109 and name HB2 ))
(( segid "PROT" and resid 21 and name HG2% ))
2.800 2.000 2.000 peak 19442 weight 0.10000E+01 volume 0.19394E+01 ppm1 1.585 ppm2 1.016
ASSI {19452}
(( segid "PROT" and resid 102 and name HD2% ))
(( segid "PROT" and resid 21 and name HG2% ))
2.500 2.500 2.000 peak 19452 weight 0.10000E+01 volume 0.38076E+01 ppm1 0.762 ppm2 1.024
ASSI {19492}
(( segid "PROT" and resid 33 and name HA ))
(( segid "PROT" and resid 33 and name HG1 ))
3.400 2.900 2.100 peak 19492 weight 0.10000E+01 volume 0.66660E+00 ppm1 3.992 ppm2 0.280
ASSI {19532}
(( segid "PROT" and resid 33 and name HB1 ))
(( segid "PROT" and resid 33 and name HG1 ))
3.300 2.700 2.200 peak 19532 weight 0.10000E+01 volume 0.76740E+00 ppm1 1.075 ppm2 0.269
ASSI {19552}
(( segid "PROT" and resid 53 and name HG2 ))
(( segid "PROT" and resid 53 and name HD1 ))
2.500 1.600 1.600 peak 19552 weight 0.10000E+01 volume 0.38667E+01 ppm1 1.948 ppm2 3.649
ASSI {19582}
(( segid "PROT" and resid 50 and name HG2% ))
(( segid "PROT" and resid 53 and name HG1 ))
3.200 2.600 2.300 peak 19582 weight 0.10000E+01 volume 0.89220E+00 ppm1 0.421 ppm2 2.280
ASSI {19602}
(( segid "PROT" and resid 53 and name HA ))

```

```

(( segid "PROT" and resid 53 and name HG1 ))
2.500 1.600 1.600 peak 19602 weight 0.10000E+01 volume 0.43485E+01 ppm1 4.119 ppm2 2.264
ASSI {19612}
(( segid "PROT" and resid 53 and name HA ))
(( segid "PROT" and resid 53 and name HD1 ))
3.200 2.600 2.300 peak 19612 weight 0.10000E+01 volume 0.92980E+00 ppm1 4.123 ppm2 3.649
ASSI {19622}
(( segid "PROT" and resid 53 and name HA ))
(( segid "PROT" and resid 53 and name HD2 ))
3.200 2.600 2.300 peak 19622 weight 0.10000E+01 volume 0.91130E+00 ppm1 4.123 ppm2 3.446
ASSI {19652}
(( segid "PROT" and resid 53 and name HG2 ))
(( segid "PROT" and resid 53 and name HB1 ))
2.000 1.000 1.000 peak 19652 weight 0.10000E+01 volume 0.15739E+02 ppm1 1.936 ppm2 2.247
ASSI {19662}
(( segid "PROT" and resid 53 and name HD1 ))
(( segid "PROT" and resid 53 and name HB1 ))
2.900 2.100 2.100 peak 19662 weight 0.10000E+01 volume 0.16703E+01 ppm1 3.652 ppm2 2.249
ASSI {19692}
(( segid "PROT" and resid 57 and name HE2 ))
(( segid "PROT" and resid 57 and name HD1 ))
2.100 1.100 1.100 peak 19692 weight 0.10000E+01 volume 0.11051E+02 ppm1 2.082 ppm2 1.752
ASSI {19732}
(( segid "PROT" and resid 21 and name HG11 ))
(( segid "PROT" and resid 17 and name HG2 ))
2.700 1.800 1.800 peak 19732 weight 0.10000E+01 volume 0.24805E+01 ppm1 1.783 ppm2 1.175
ASSI {19762}
(( segid "PROT" and resid 17 and name HB ))
(( segid "PROT" and resid 17 and name HG2 ))
2.000 1.000 1.000 peak 19762 weight 0.10000E+01 volume 0.16615E+02 ppm1 4.290 ppm2 1.178
ASSI {19772}
(( segid "PROT" and resid 102 and name HD2 ))
(( segid "PROT" and resid 25 and name HG2 ))
2.000 1.000 1.000 peak 19772 weight 0.10000E+01 volume 0.16186E+02 ppm1 0.763 ppm2 1.073
ASSI {19812}
(( segid "PROT" and resid 31 and name HB ))
(( segid "PROT" and resid 25 and name HG2 ))
2.400 1.400 1.400 peak 19812 weight 0.10000E+01 volume 0.53511E+01 ppm1 1.761 ppm2 1.082
ASSI {19852}
(( segid "PROT" and resid 57 and name HE2 ))
(( segid "PROT" and resid 58 and name HG2 ))
2.600 1.700 1.700 peak 19852 weight 0.10000E+01 volume 0.33672E+01 ppm1 2.081 ppm2 1.095
ASSI {19862}
(( segid "PROT" and resid 54 and name HE ))
(( segid "PROT" and resid 58 and name HG2 ))
2.100 1.100 1.100 peak 19862 weight 0.10000E+01 volume 0.11606E+02 ppm1 2.004 ppm2 1.097
ASSI {19912}
(( segid "PROT" and resid 57 and name HE1 ))
(( segid "PROT" and resid 57 and name HB2 ))
3.400 2.900 2.100 peak 19912 weight 0.10000E+01 volume 0.69760E+00 ppm1 2.617 ppm2 1.141
ASSI {19922}
(( segid "PROT" and resid 57 and name HD1 ))
(( segid "PROT" and resid 57 and name HB2 ))
3.200 2.600 2.300 peak 19922 weight 0.10000E+01 volume 0.95330E+00 ppm1 1.757 ppm2 1.144
ASSI {19952}
(( segid "PROT" and resid 96 and name HB1 ))
(( segid "PROT" and resid 91 and name HA ))
3.100 2.400 2.400 peak 19952 weight 0.10000E+01 volume 0.10916E+01 ppm1 3.416 ppm2 2.586
ASSI {19982}
(( segid "PROT" and resid 91 and name HA ))
(( segid "PROT" and resid 91 and name HB1 ))
2.300 1.300 1.300 peak 19982 weight 0.10000E+01 volume 0.66821E+01 ppm1 2.590 ppm2 1.625
ASSI {19992}
(( segid "PROT" and resid 91 and name HA ))
(( segid "PROT" and resid 91 and name HG1 ))
3.100 2.400 2.400 peak 19992 weight 0.10000E+01 volume 0.12229E+01 ppm1 2.589 ppm2 1.994
ASSI {20022}
(( segid "PROT" and resid 8 and name HB2 ))
(( segid "PROT" and resid 8 and name HD1 ))
3.000 2.200 2.200 peak 20022 weight 0.10000E+01 volume 0.14969E+01 ppm1 1.927 ppm2 3.869
ASSI {20052}
(( segid "PROT" and resid 90 and name HA ))
(( segid "PROT" and resid 90 and name HB2 ))
3.100 2.400 2.400 peak 20052 weight 0.10000E+01 volume 0.11109E+01 ppm1 4.645 ppm2 2.168
ASSI {20062}
(( segid "PROT" and resid 90 and name HA ))
(( segid "PROT" and resid 90 and name HB1 ))
3.000 2.200 2.200 peak 20062 weight 0.10000E+01 volume 0.14418E+01 ppm1 4.643 ppm2 2.353
ASSI {20082}
(( segid "PROT" and resid 90 and name HD2 ))
(( segid "PROT" and resid 90 and name HB1 ))
3.200 2.600 2.300 peak 20082 weight 0.10000E+01 volume 0.91280E+00 ppm1 3.930 ppm2 2.351
ASSI {20182}
(( segid "PROT" and resid 30 and name HB2 ))
(( segid "PROT" and resid 102 and name HD1 ))
2.800 2.000 2.000 peak 20182 weight 0.10000E+01 volume 0.21637E+01 ppm1 3.970 ppm2 0.761
ASSI {20252}
(( segid "PROT" and resid 28 and name HD2 ))
(( segid "PROT" and resid 28 and name HA ))

```

3.100	2.400	2.400	peak 20252 weight	0.10000E+01 volume	0.11231E+01 ppm1	5.008 ppm2	4.019
ASSI {20282}							
((segid "PROT" and resid 32 and name HE3))							
((segid "PROT" and resid 32 and name HB2))							
3.000	2.200	2.200	peak 20282 weight	0.10000E+01 volume	0.13378E+01 ppm1	7.355 ppm2	3.414
ASSI {20292}							
((segid "PROT" and resid 32 and name HE3))							
((segid "PROT" and resid 32 and name HB1))							
3.000	2.200	2.200	peak 20292 weight	0.10000E+01 volume	0.13945E+01 ppm1	7.357 ppm2	3.634
ASSI {20302}							
((segid "PROT" and resid 32 and name HD1))							
((segid "PROT" and resid 32 and name HB1))							
3.300	2.700	2.200	peak 20302 weight	0.10000E+01 volume	0.86510E+00 ppm1	7.888 ppm2	3.645
ASSI {20312}							
((segid "PROT" and resid 32 and name HD1))							
((segid "PROT" and resid 32 and name HB2))							
3.000	2.200	2.200	peak 20312 weight	0.10000E+01 volume	0.13496E+01 ppm1	7.887 ppm2	3.406
ASSI {20322}							
((segid "PROT" and resid 32 and name HD1))							
((segid "PROT" and resid 30 and name HA))							
3.300	2.700	2.200	peak 20322 weight	0.10000E+01 volume	0.84000E+00 ppm1	7.887 ppm2	4.846
ASSI {20332}							
((segid "PROT" and resid 75 and name HA))							
((segid "PROT" and resid 74 and name HB1))							
2.800	2.000	2.000	peak 20332 weight	0.10000E+01 volume	0.19988E+01 ppm1	4.058 ppm2	3.004
ASSI {20342}							
((segid "PROT" and resid 82 and name HE%))							
((segid "PROT" and resid 82 and name HB1))							
3.500	3.100	2.000	peak 20342 weight	0.10000E+01 volume	0.58330E+00 ppm1	6.488 ppm2	3.143
ASSI {20382}							
((segid "PROT" and resid 105 and name HD%))							
((segid "PROT" and resid 105 and name HB1))							
2.600	1.700	1.700	peak 20382 weight	0.10000E+01 volume	0.35159E+01 ppm1	7.235 ppm2	3.138
ASSI {20412}							
((segid "PROT" and resid 107 and name HD%))							
((segid "PROT" and resid 107 and name HB1))							
2.500	1.600	1.600	peak 20412 weight	0.10000E+01 volume	0.39879E+01 ppm1	7.241 ppm2	3.090
ASSI {20432}							
((segid "PROT" and resid 96 and name HD%))							
((segid "PROT" and resid 96 and name HA))							
3.200	2.600	2.300	peak 20432 weight	0.10000E+01 volume	0.10372E+01 ppm1	7.151 ppm2	3.826
ASSI {20462}							
((segid "PROT" and resid 47 and name HD%))							
((segid "PROT" and resid 47 and name HB1))							
2.900	2.100	2.100	peak 20462 weight	0.10000E+01 volume	0.18851E+01 ppm1	7.401 ppm2	3.245
ASSI {20472}							
((segid "PROT" and resid 47 and name HD%))							
((segid "PROT" and resid 47 and name HB2))							
3.000	2.200	2.200	peak 20472 weight	0.10000E+01 volume	0.13814E+01 ppm1	7.409 ppm2	2.843
ASSI {20482}							
((segid "PROT" and resid 47 and name HE%))							
((segid "PROT" and resid 47 and name HB1))							
3.400	2.900	2.100	peak 20482 weight	0.10000E+01 volume	0.68190E+00 ppm1	6.688 ppm2	3.236
ASSI {20492}							
((segid "PROT" and resid 47 and name HE%))							
((segid "PROT" and resid 47 and name HB2))							
3.500	3.100	2.000	peak 20492 weight	0.10000E+01 volume	0.54300E+00 ppm1	6.675 ppm2	2.861
ASSI {20502}							
((segid "PROT" and resid 47 and name HE%))							
((segid "PROT" and resid 47 and name HA))							
3.300	2.700	2.200	peak 20502 weight	0.10000E+01 volume	0.81170E+00 ppm1	6.675 ppm2	4.131
ASSI {20512}							
((segid "PROT" and resid 15 and name HE%))							
((segid "PROT" and resid 15 and name HA))							
3.400	2.900	2.100	peak 20512 weight	0.10000E+01 volume	0.67340E+00 ppm1	6.926 ppm2	4.050
ASSI {20522}							
((segid "PROT" and resid 67 and name HE%))							
((segid "PROT" and resid 67 and name HA))							
3.300	2.700	2.200	peak 20522 weight	0.10000E+01 volume	0.82160E+00 ppm1	6.735 ppm2	4.108
ASSI {20532}							
((segid "PROT" and resid 67 and name HE%))							
((segid "PROT" and resid 67 and name HB2))							
3.700	3.400	1.800	peak 20532 weight	0.10000E+01 volume	0.39270E+00 ppm1	6.737 ppm2	2.093
ASSI {20542}							
((segid "PROT" and resid 67 and name HE%))							
((segid "PROT" and resid 67 and name HB1))							
3.400	2.900	2.100	peak 20542 weight	0.10000E+01 volume	0.68200E+00 ppm1	6.737 ppm2	3.003
ASSI {20552}							
((segid "PROT" and resid 68 and name HE%))							
((segid "PROT" and resid 68 and name HA))							
3.200	2.600	2.300	peak 20552 weight	0.10000E+01 volume	0.96420E+00 ppm1	7.310 ppm2	4.583
ASSI {20582}							
((segid "PROT" and resid 67 and name HA))							
((segid "PROT" and resid 68 and name HA))							
3.000	2.200	2.200	peak 20582 weight	0.10000E+01 volume	0.13549E+01 ppm1	4.106 ppm2	4.583
ASSI {20602}							
((segid "PROT" and resid 68 and name HD%))							
((segid "PROT" and resid 68 and name HB2))							
3.000	2.200	2.200	peak 20602 weight	0.10000E+01 volume	0.14100E+01 ppm1	7.209 ppm2	2.960

```

ASSI {20612}
( segid "PROT" and resid 68 and name HD% )
(( segid "PROT" and resid 68 and name HB1 ))
2.900 2.100 2.100 peak 20612 weight 0.10000E+01 volume 0.15572E+01 ppm1 7.209 ppm2 3.104
ASSI {20622}
( segid "PROT" and resid 68 and name HE% )
(( segid "PROT" and resid 68 and name HB2 ))
3.200 2.600 2.300 peak 20622 weight 0.10000E+01 volume 0.95790E+00 ppm1 7.315 ppm2 2.958
ASSI {20632}
( segid "PROT" and resid 68 and name HE% )
(( segid "PROT" and resid 68 and name HB1 ))
3.300 2.700 2.200 peak 20632 weight 0.10000E+01 volume 0.77790E+00 ppm1 7.316 ppm2 3.095
ASSI {20642}
( segid "PROT" and resid 88 and name HE% )
(( segid "PROT" and resid 88 and name HA ))
3.300 2.700 2.200 peak 20642 weight 0.10000E+01 volume 0.74810E+00 ppm1 6.652 ppm2 4.331
ASSI {20652}
( segid "PROT" and resid 50 and name HD1% )
(( segid "PROT" and resid 88 and name HA ))
3.300 2.700 2.200 peak 20652 weight 0.10000E+01 volume 0.73730E+00 ppm1 0.582 ppm2 4.313
ASSI {20732}
( segid "PROT" and resid 96 and name HD% )
(( segid "PROT" and resid 96 and name HB1 ))
3.000 2.200 2.200 peak 20732 weight 0.10000E+01 volume 0.12722E+01 ppm1 7.122 ppm2 3.421
ASSI {20742}
( segid "PROT" and resid 96 and name HE% )
(( segid "PROT" and resid 96 and name HB2 ))
3.200 2.600 2.300 peak 20742 weight 0.10000E+01 volume 0.10176E+01 ppm1 7.054 ppm2 2.580
ASSI {20752}
( segid "PROT" and resid 96 and name HE% )
(( segid "PROT" and resid 96 and name HB1 ))
3.200 2.600 2.300 peak 20752 weight 0.10000E+01 volume 0.98070E+00 ppm1 7.054 ppm2 3.429
ASSI {20762}
( segid "PROT" and resid 96 and name HE% )
(( segid "PROT" and resid 96 and name HA ))
3.200 2.600 2.300 peak 20762 weight 0.10000E+01 volume 0.10206E+01 ppm1 7.054 ppm2 3.823
ASSI {20792}
( segid "PROT" and resid 99 and name HB% )
( segid "PROT" and resid 81 and name HG2% )
3.100 2.400 2.400 peak 20792 weight 0.10000E+01 volume 0.12313E+01 ppm1 1.655 ppm2 0.157
ASSI {20812}
(( segid "PROT" and resid 44 and name HG2 ))
(( segid "PROT" and resid 43 and name HA ))
3.300 2.700 2.200 peak 20812 weight 0.10000E+01 volume 0.81200E+00 ppm1 2.075 ppm2 4.987
ASSI {20822}
( segid "PROT" and resid 46 and name HE% )
( segid "PROT" and resid 43 and name HB% )
3.100 2.400 2.400 peak 20822 weight 0.10000E+01 volume 0.11247E+01 ppm1 5.998 ppm2 0.978
ASSI {20832}
(( segid "PROT" and resid 39 and name HE2 ))
( segid "PROT" and resid 43 and name HB% )
3.100 2.400 2.400 peak 20832 weight 0.10000E+01 volume 0.12227E+01 ppm1 2.950 ppm2 0.972
ASSI {20842}
(( segid "PROT" and resid 61 and name HB2 ))
(( segid "PROT" and resid 58 and name HA ))
3.100 2.400 2.400 peak 20842 weight 0.10000E+01 volume 0.12246E+01 ppm1 2.120 ppm2 3.883
ASSI {20862}
(( segid "PROT" and resid 70 and name HB1 ))
( segid "PROT" and resid 69 and name HG2% )
2.800 2.000 2.000 peak 20862 weight 0.10000E+01 volume 0.20271E+01 ppm1 4.227 ppm2 0.859
ASSI {20872}
(( segid "PROT" and resid 110 and name HG12 ))
(( segid "PROT" and resid 107 and name HA ))
2.600 1.700 1.700 peak 20872 weight 0.10000E+01 volume 0.36962E+01 ppm1 1.090 ppm2 3.857
ASSI {20992}
(( segid "PROT" and resid 79 and name HB2 ))
( segid "PROT" and resid 83 and name HG2% )
3.200 2.600 2.300 peak 20992 weight 0.10000E+01 volume 0.96340E+00 ppm1 2.102 ppm2 1.343
ASSI {21032}
(( segid "PROT" and resid 68 and name HB2 ))
( segid "PROT" and resid 63 and name HD2% )
3.100 2.400 2.400 peak 21032 weight 0.10000E+01 volume 0.12579E+01 ppm1 2.956 ppm2 1.082
ASSI {21062}
(( segid "PROT" and resid 116 and name HA ))
( segid "PROT" and resid 110 and name HD1% )
3.300 2.700 2.200 peak 21062 weight 0.10000E+01 volume 0.75760E+00 ppm1 4.275 ppm2 0.571
ASSI {21102}
(( segid "PROT" and resid 75 and name HG1 ))
( segid "PROT" and resid 116 and name HD1% )
3.100 2.400 2.400 peak 21102 weight 0.10000E+01 volume 0.12677E+01 ppm1 2.317 ppm2 0.825
ASSI {21172}
(( segid "PROT" and resid 97 and name HG2 ))
( segid "PROT" and resid 101 and name HD1% )
3.100 2.400 2.400 peak 21172 weight 0.10000E+01 volume 0.11617E+01 ppm1 1.617 ppm2 0.997
ASSI {21222}
(( segid "PROT" and resid 30 and name HE2 ))
( segid "PROT" and resid 101 and name HD1% )
3.300 2.700 2.200 peak 21222 weight 0.10000E+01 volume 0.83430E+00 ppm1 3.976 ppm2 0.993
ASSI {21242}

```



```

(( segid "PROT" and resid 59 and name HG1 ))
( segid "PROT" and resid 54 and name HE% )
2.800 2.000 2.000 peak 21242 weight 0.10000E+01 volume 0.19137E+01 ppm1 2.624 ppm2 2.002
ASSI {21312}
(( segid "PROT" and resid 56 and name HA ))
( segid "PROT" and resid 59 and name HE% )
3.300 2.700 2.200 peak 21312 weight 0.10000E+01 volume 0.81010E+00 ppm1 4.056 ppm2 1.308
ASSI {21382}
(( segid "PROT" and resid 116 and name HG12 ))
( segid "PROT" and resid 75 and name HE% )
3.600 3.200 1.900 peak 21382 weight 0.10000E+01 volume 0.47290E+00 ppm1 0.970 ppm2 2.096
ASSI {21432}
( segid "PROT" and resid 25 and name HG1% )
( segid "PROT" and resid 21 and name HG2% )
2.100 1.100 1.100 peak 21432 weight 0.10000E+01 volume 0.11034E+02 ppm1 1.244 ppm2 1.023
ASSI {21442}
(( segid "PROT" and resid 25 and name HB ))
( segid "PROT" and resid 21 and name HG2% )
3.200 2.600 2.300 peak 21442 weight 0.10000E+01 volume 0.97890E+00 ppm1 2.446 ppm2 1.018
ASSI {21512}
(( segid "PROT" and resid 116 and name HG12 ))
( segid "PROT" and resid 116 and name HG2% )
2.300 1.300 1.300 peak 21512 weight 0.10000E+01 volume 0.68119E+01 ppm1 0.986 ppm2 0.854
ASSI {21552}
(( segid "PROT" and resid 105 and name HB1 ))
( segid "PROT" and resid 101 and name HG2% )
3.100 2.400 2.400 peak 21552 weight 0.10000E+01 volume 0.10529E+01 ppm1 3.188 ppm2 1.032
ASSI {21632}
( segid "PROT" and resid 73 and name HD2% )
( segid "PROT" and resid 76 and name HB% )
2.700 1.800 1.800 peak 21632 weight 0.10000E+01 volume 0.27029E+01 ppm1 0.929 ppm2 1.533
ASSI {21662}
(( segid "PROT" and resid 79 and name HB1 ))
( segid "PROT" and resid 76 and name HB% )
3.100 2.400 2.400 peak 21662 weight 0.10000E+01 volume 0.11536E+01 ppm1 2.220 ppm2 1.530
ASSI {21672}
(( segid "PROT" and resid 79 and name HB2 ))
( segid "PROT" and resid 76 and name HB% )
3.300 2.700 2.200 peak 21672 weight 0.10000E+01 volume 0.84220E+00 ppm1 2.111 ppm2 1.529
ASSI {21682}
(( segid "PROT" and resid 80 and name HB2 ))
( segid "PROT" and resid 76 and name HB% )
3.100 2.400 2.400 peak 21682 weight 0.10000E+01 volume 0.12504E+01 ppm1 1.938 ppm2 1.531
ASSI {21692}
(( segid "PROT" and resid 80 and name HB1 ))
( segid "PROT" and resid 76 and name HB% )
3.100 2.400 2.400 peak 21692 weight 0.10000E+01 volume 0.10520E+01 ppm1 2.003 ppm2 1.531
ASSI {21732}
(( segid "PROT" and resid 100 and name HA ))
( segid "PROT" and resid 99 and name HB% )
3.000 2.200 2.200 peak 21732 weight 0.10000E+01 volume 0.12872E+01 ppm1 4.363 ppm2 1.659
ASSI {21752}
( segid "PROT" and resid 82 and name HE% )
( segid "PROT" and resid 99 and name HB% )
3.200 2.600 2.300 peak 21752 weight 0.10000E+01 volume 0.93520E+00 ppm1 6.489 ppm2 1.660
ASSI {21762}
( segid "PROT" and resid 34 and name HE% )
( segid "PROT" and resid 99 and name HB% )
3.200 2.600 2.300 peak 21762 weight 0.10000E+01 volume 0.10406E+01 ppm1 7.173 ppm2 1.663
ASSI {21772}
( segid "PROT" and resid 68 and name HE% )
( segid "PROT" and resid 76 and name HB% )
3.200 2.600 2.300 peak 21772 weight 0.10000E+01 volume 0.88080E+00 ppm1 7.319 ppm2 1.535
ASSI {21922}
(( segid "PROT" and resid 14 and name HA ))
( segid "PROT" and resid 113 and name HB% )
3.200 2.600 2.300 peak 21922 weight 0.10000E+01 volume 0.10349E+01 ppm1 4.100 ppm2 1.406
ASSI {21952}
(( segid "PROT" and resid 33 and name HG1 ))
( segid "PROT" and resid 31 and name HB% )
3.500 3.100 2.000 peak 21952 weight 0.10000E+01 volume 0.53810E+00 ppm1 0.265 ppm2 1.760
ASSI {21962}
( segid "PROT" and resid 56 and name HD2% )
( segid "PROT" and resid 31 and name HB% )
3.300 2.700 2.200 peak 21962 weight 0.10000E+01 volume 0.75920E+00 ppm1 0.678 ppm2 1.762
ASSI {21972}
(( segid "PROT" and resid 34 and name HN ))
( segid "PROT" and resid 31 and name HB% )
3.700 3.400 1.800 peak 21972 weight 0.10000E+01 volume 0.42810E+00 ppm1 7.588 ppm2 1.760
ASSI {21992}
(( segid "PROT" and resid 42 and name HB1 ))
( segid "PROT" and resid 43 and name HB% )
3.200 2.600 2.300 peak 21992 weight 0.10000E+01 volume 0.89240E+00 ppm1 2.221 ppm2 0.984
ASSI {22022}
(( segid "PROT" and resid 87 and name HG2 ))
( segid "PROT" and resid 49 and name HG2% )
3.100 2.400 2.400 peak 22022 weight 0.10000E+01 volume 0.10861E+01 ppm1 2.245 ppm2 0.910
ASSI {22032}
(( segid "PROT" and resid 39 and name HA ))

```

```

( segid "PROT" and resid 38 and name HG2%)
3.600 3.200 1.900 peak 22032 weight 0.10000E+01 volume 0.44230E+00 ppm1 4.441 ppm2 -0.010
ASSI {22052}
( segid "PROT" and resid 18 and name HD1%)
( segid "PROT" and resid 69 and name HG1%)
3.500 3.100 2.000 peak 22052 weight 0.10000E+01 volume 0.55350E+00 ppm1 0.503 ppm2 0.989
ASSI {22062}
(( segid "PROT" and resid 68 and name HA ))
( segid "PROT" and resid 69 and name HG1%)
3.400 2.900 2.100 peak 22062 weight 0.10000E+01 volume 0.63530E+00 ppm1 4.580 ppm2 0.991
ASSI {22072}
(( segid "PROT" and resid 33 and name HB1 ))
( segid "PROT" and resid 81 and name HG2%)
3.500 3.100 2.000 peak 22072 weight 0.10000E+01 volume 0.57540E+00 ppm1 1.066 ppm2 0.155
ASSI {22092}
(( segid "PROT" and resid 77 and name HA ))
( segid "PROT" and resid 81 and name HG1%)
3.600 3.200 1.900 peak 22092 weight 0.10000E+01 volume 0.47080E+00 ppm1 4.407 ppm2 0.510
ASSI {22152}
(( segid "PROT" and resid 106 and name HB2 ))
( segid "PROT" and resid 25 and name HG2%)
3.300 2.700 2.200 peak 22152 weight 0.10000E+01 volume 0.76240E+00 ppm1 3.135 ppm2 1.076
ASSI {22192}
(( segid "PROT" and resid 42 and name HA ))
( segid "PROT" and resid 41 and name HG2%)
3.200 2.600 2.300 peak 22192 weight 0.10000E+01 volume 0.91170E+00 ppm1 4.500 ppm2 1.320
ASSI {22312}
(( segid "PROT" and resid 56 and name HB2 ))
( segid "PROT" and resid 22 and name HD2%)
3.000 2.200 2.200 peak 22312 weight 0.10000E+01 volume 0.13684E+01 ppm1 1.428 ppm2 1.049
ASSI {22342}
(( segid "PROT" and resid 60 and name HA ))
( segid "PROT" and resid 22 and name HD2%)
3.500 3.100 2.000 peak 22342 weight 0.10000E+01 volume 0.54580E+00 ppm1 4.434 ppm2 1.047
ASSI {22362}
( segid "PROT" and resid 31 and name HB%)
( segid "PROT" and resid 102 and name HD2%)
2.300 1.300 1.300 peak 22362 weight 0.10000E+01 volume 0.61478E+01 ppm1 1.763 ppm2 0.768
ASSI {22422}
(( segid "PROT" and resid 106 and name HB2 ))
( segid "PROT" and resid 78 and name HD2%)
3.300 2.700 2.200 peak 22422 weight 0.10000E+01 volume 0.75770E+00 ppm1 3.129 ppm2 0.196
ASSI {22432}
(( segid "PROT" and resid 103 and name HA ))
( segid "PROT" and resid 102 and name HD2%)
2.700 1.800 1.800 peak 22432 weight 0.10000E+01 volume 0.25754E+01 ppm1 3.195 ppm2 0.766
ASSI {22482}
( segid "PROT" and resid 82 and name HE%)
( segid "PROT" and resid 102 and name HD2%)
2.800 2.000 2.000 peak 22482 weight 0.10000E+01 volume 0.19487E+01 ppm1 6.468 ppm2 0.763
ASSI {22552}
( segid "PROT" and resid 56 and name HD1%)
( segid "PROT" and resid 102 and name HD1%)
2.500 1.600 1.600 peak 22552 weight 0.10000E+01 volume 0.45008E+01 ppm1 0.986 ppm2 0.760
ASSI {22582}
(( segid "PROT" and resid 34 and name HB2 ))
( segid "PROT" and resid 102 and name HD1%)
3.400 2.900 2.100 peak 22582 weight 0.10000E+01 volume 0.62740E+00 ppm1 2.649 ppm2 0.760
ASSI {22612}
(( segid "PROT" and resid 101 and name HA ))
( segid "PROT" and resid 104 and name HG1 ))
2.900 2.100 2.100 peak 22612 weight 0.10000E+01 volume 0.16583E+01 ppm1 3.706 ppm2 1.550
ASSI {22652}
( segid "PROT" and resid 63 and name HD1%)
( segid "PROT" and resid 66 and name HB2 ))
3.600 3.200 1.900 peak 22652 weight 0.10000E+01 volume 0.45770E+00 ppm1 0.917 ppm2 2.048
ASSI {22712}
(( segid "PROT" and resid 74 and name HA ))
( segid "PROT" and resid 18 and name HD1%)
3.200 2.600 2.300 peak 22712 weight 0.10000E+01 volume 0.97160E+00 ppm1 3.804 ppm2 0.514
ASSI {22722}
(( segid "PROT" and resid 68 and name HA ))
( segid "PROT" and resid 18 and name HD1%)
3.400 2.900 2.100 peak 22722 weight 0.10000E+01 volume 0.62210E+00 ppm1 4.578 ppm2 0.514
ASSI {22752}
(( segid "PROT" and resid 33 and name HB1 ))
(( segid "PROT" and resid 33 and name HG2 ))
3.500 3.100 2.000 peak 22752 weight 0.10000E+01 volume 0.57510E+00 ppm1 1.036 ppm2 -0.870
ASSI {22772}
(( segid "PROT" and resid 98 and name HB1 ))
(( segid "PROT" and resid 33 and name HG1 ))
3.300 2.700 2.200 peak 22772 weight 0.10000E+01 volume 0.77490E+00 ppm1 3.392 ppm2 0.271
ASSI {22792}
(( segid "PROT" and resid 34 and name HZ ))
(( segid "PROT" and resid 33 and name HG1 ))
3.200 2.600 2.300 peak 22792 weight 0.10000E+01 volume 0.90520E+00 ppm1 7.250 ppm2 0.266
ASSI {22802}
(( segid "PROT" and resid 70 and name HA ))
( segid "PROT" and resid 14 and name HD1%)

```

2.600	1.700	1.700	peak 22802	weight 0.10000E+01	volume 0.33402E+01	ppm1 4.795	ppm2 0.855	
ASSI {22842}								
((segid "PROT" and resid 59 and name HE%))								
((segid "PROT" and resid 78 and name HD1%))								
2.500	1.600	1.600	peak 22842	weight 0.10000E+01	volume 0.45695E+01	ppm1 1.310	ppm2 0.094	
ASSI {22932}								
((segid "PROT" and resid 60 and name HA))								
((segid "PROT" and resid 22 and name HD1%))								
3.000	2.200	2.200	peak 22932	weight 0.10000E+01	volume 0.14457E+01	ppm1 4.433	ppm2 1.106	
ASSI {23032}								
((segid "PROT" and resid 35 and name HG1))								
((segid "PROT" and resid 56 and name HD1%))								
3.200	2.600	2.300	peak 23032	weight 0.10000E+01	volume 0.96100E+00	ppm1 2.893	ppm2 0.977	
ASSI {23122}								
((segid "PROT" and resid 78 and name HN))								
((segid "PROT" and resid 78 and name HG))								
3.600	3.200	1.900	peak 23122	weight 0.10000E+01	volume 0.50520E+00	ppm1 7.384	ppm2 0.692	
ASSI {23152}								
((segid "PROT" and resid 44 and name HG1))								
((segid "PROT" and resid 44 and name HG2))								
1.800	0.800	0.800	peak 23152	weight 0.10000E+01	volume 0.30462E+02	ppm1 2.203	ppm2 2.079	
ASSI {23202}								
((segid "PROT" and resid 52 and name HA))								
((segid "PROT" and resid 53 and name HG2))								
3.400	2.900	2.100	peak 23202	weight 0.10000E+01	volume 0.70630E+00	ppm1 5.047	ppm2 1.939	
ASSI {23252}								
((segid "PROT" and resid 35 and name HN))								
((segid "PROT" and resid 32 and name HB2))								
3.500	3.100	2.000	peak 23252	weight 0.10000E+01	volume 0.53670E+00	ppm1 7.151	ppm2 3.408	
ASSI {23312}								
((segid "PROT" and resid 21 and name HA))								
((segid "PROT" and resid 24 and name HB1))								
3.000	2.200	2.200	peak 23312	weight 0.10000E+01	volume 0.14681E+01	ppm1 3.796	ppm2 2.501	
ASSI {23362}								
((segid "PROT" and resid 9 and name HD1))								
((segid "PROT" and resid 7 and name HB2))								
2.700	1.800	1.800	peak 23362	weight 0.10000E+01	volume 0.26162E+01	ppm1 3.211	ppm2 1.943	
ASSI {23422}								
((segid "PROT" and resid 52 and name HA))								
((segid "PROT" and resid 51 and name HB2))								
3.500	3.100	2.000	peak 23422	weight 0.10000E+01	volume 0.55120E+00	ppm1 5.036	ppm2 1.214	
ASSI {23442}								
((segid "PROT" and resid 82 and name HD%))								
((segid "PROT" and resid 81 and name HB))								
3.400	2.900	2.100	peak 23442	weight 0.10000E+01	volume 0.63500E+00	ppm1 6.702	ppm2 1.465	
ASSI {23452}								
((segid "PROT" and resid 54 and name HB2))								
((segid "PROT" and resid 54 and name HG2))								
2.800	2.000	2.000	peak 23452	weight 0.10000E+01	volume 0.23115E+01	ppm1 1.379	ppm2 1.886	
ASSI {23682}								
((segid "PROT" and resid 10 and name HA))								
((segid "PROT" and resid 11 and name HB1))								
3.300	2.700	2.200	peak 23682	weight 0.10000E+01	volume 0.74660E+00	ppm1 4.909	ppm2 2.381	
ASSI {23692}								
((segid "PROT" and resid 34 and name HA))								
((segid "PROT" and resid 35 and name HB2))								
3.400	2.900	2.100	peak 23692	weight 0.10000E+01	volume 0.63830E+00	ppm1 5.015	ppm2 2.239	
ASSI {23742}								
((segid "PROT" and resid 110 and name HG2%))								
((segid "PROT" and resid 75 and name HB2))								
3.300	2.700	2.200	peak 23742	weight 0.10000E+01	volume 0.81390E+00	ppm1 0.689	ppm2 2.656	
ASSI {23802}								
((segid "PROT" and resid 74 and name HD%))								
((segid "PROT" and resid 75 and name HB1))								
3.300	2.700	2.200	peak 23802	weight 0.10000E+01	volume 0.82510E+00	ppm1 6.425	ppm2 2.966	
ASSI {23822}								
((segid "PROT" and resid 29 and name HE21))								
((segid "PROT" and resid 29 and name HG2))								
3.300	2.700	2.200	peak 23822	weight 0.10000E+01	volume 0.78340E+00	ppm1 7.587	ppm2 2.428	
ASSI {23832}								
((segid "PROT" and resid 29 and name HE21))								
((segid "PROT" and resid 29 and name HG1))								
3.400	2.900	2.100	peak 23832	weight 0.10000E+01	volume 0.64100E+00	ppm1 7.588	ppm2 2.492	
ASSI {23842}								
((segid "PROT" and resid 50 and name HA))								
((segid "PROT" and resid 49 and name HB))								
2.800	2.000	2.000	peak 23842	weight 0.10000E+01	volume 0.19918E+01	ppm1 3.934	ppm2 1.925	
ASSI {23862}								
((segid "PROT" and resid 88 and name HB1))								
((segid "PROT" and resid 49 and name HB))								
3.300	2.700	2.200	peak 23862	weight 0.10000E+01	volume 0.73730E+00	ppm1 2.966	ppm2 1.926	
ASSI {23882}								
((segid "PROT" and resid 87 and name HG2))								
((segid "PROT" and resid 49 and name HB))								
2.800	2.000	2.000	peak 23882	weight 0.10000E+01	volume 0.22351E+01	ppm1 2.214	ppm2 1.924	
ASSI {23892}								
((segid "PROT" and resid 50 and name HG11))								
((segid "PROT" and resid 49 and name HB))								
3.500	3.100	2.000	peak 23892	weight 0.10000E+01	volume 0.55230E+00	ppm1 0.800	ppm2 1.928	

```

ASSI {23932}
  (( segid "PROT" and resid 19 and name HG1 ))
  (( segid "PROT" and resid 23 and name HG2 ))
  3.500 3.100 2.000 peak 23932 weight 0.10000E+01 volume 0.58220E+00 ppm1 1.292 ppm2 2.484
ASSI {24002}
  (( segid "PROT" and resid 111 and name HG2 ))
  (( segid "PROT" and resid 112 and name HG2 ))
  3.400 2.900 2.100 peak 24002 weight 0.10000E+01 volume 0.70990E+00 ppm1 1.339 ppm2 2.254
ASSI {24032}
  (( segid "PROT" and resid 116 and name HD1% ))
  (( segid "PROT" and resid 110 and name HB ))
  3.200 2.600 2.300 peak 24032 weight 0.10000E+01 volume 0.89320E+00 ppm1 0.840 ppm2 1.796
ASSI {24052}
  (( segid "PROT" and resid 92 and name HB1 ))
  (( segid "PROT" and resid 92 and name HG2 ))
  2.000 1.000 1.000 peak 24052 weight 0.10000E+01 volume 0.15248E+02 ppm1 2.094 ppm2 2.263
ASSI {24062}
  (( segid "PROT" and resid 92 and name HB1 ))
  (( segid "PROT" and resid 92 and name HG1 ))
  2.000 1.000 1.000 peak 24062 weight 0.10000E+01 volume 0.14295E+02 ppm1 2.105 ppm2 2.387
ASSI {24132}
  (( segid "PROT" and resid 110 and name HG11 ))
  (( segid "PROT" and resid 107 and name HB1 ))
  3.500 3.100 2.000 peak 24132 weight 0.10000E+01 volume 0.52990E+00 ppm1 1.150 ppm2 3.098
ASSI {24152}
  (( segid "PROT" and resid 103 and name HB2 ))
  (( segid "PROT" and resid 82 and name HB1 ))
  3.300 2.700 2.200 peak 24152 weight 0.10000E+01 volume 0.85610E+00 ppm1 1.337 ppm2 3.134
ASSI {24172}
  (( segid "PROT" and resid 78 and name HD1% ))
  (( segid "PROT" and resid 106 and name HB1 ))
  3.600 3.200 1.900 peak 24172 weight 0.10000E+01 volume 0.48250E+00 ppm1 0.088 ppm2 3.343
ASSI {24202}
  (( segid "PROT" and resid 30 and name HB2 ))
  (( segid "PROT" and resid 101 and name HB ))
  3.400 2.900 2.100 peak 24202 weight 0.10000E+01 volume 0.68200E+00 ppm1 3.981 ppm2 1.942
ASSI {24212}
  (( segid "PROT" and resid 56 and name HD2% ))
  (( segid "PROT" and resid 34 and name HB2 ))
  3.400 2.900 2.100 peak 24212 weight 0.10000E+01 volume 0.65310E+00 ppm1 0.682 ppm2 2.633
ASSI {24252}
  (( segid "PROT" and resid 63 and name HD1% ))
  (( segid "PROT" and resid 18 and name HB2 ))
  3.500 3.100 2.000 peak 24252 weight 0.10000E+01 volume 0.55670E+00 ppm1 0.912 ppm2 0.346
ASSI {24272}
  (( segid "PROT" and resid 14 and name HD2% ))
  (( segid "PROT" and resid 18 and name HB1 ))
  3.300 2.700 2.200 peak 24272 weight 0.10000E+01 volume 0.73750E+00 ppm1 0.844 ppm2 1.556
ASSI {24342}
  (( segid "PROT" and resid 18 and name HD1% ))
  (( segid "PROT" and resid 14 and name HB2 ))
  3.400 2.900 2.100 peak 24342 weight 0.10000E+01 volume 0.67750E+00 ppm1 0.517 ppm2 1.595
ASSI {24372}
  (( segid "PROT" and resid 26 and name HA ))
  (( segid "PROT" and resid 56 and name HB1 ))
  3.200 2.600 2.300 peak 24372 weight 0.10000E+01 volume 0.87170E+00 ppm1 3.925 ppm2 2.094
ASSI {24382}
  (( segid "PROT" and resid 26 and name HA ))
  (( segid "PROT" and resid 56 and name HB2 ))
  3.200 2.600 2.300 peak 24382 weight 0.10000E+01 volume 0.90000E+00 ppm1 3.926 ppm2 1.456
ASSI {24402}
  (( segid "PROT" and resid 82 and name HD% ))
  (( segid "PROT" and resid 102 and name HB1 ))
  3.500 3.100 2.000 peak 24402 weight 0.10000E+01 volume 0.52400E+00 ppm1 6.701 ppm2 1.471
ASSI {24532}
  (( segid "PROT" and resid 116 and name HD1% ))
  (( segid "PROT" and resid 115 and name HB2 ))
  3.100 2.400 2.400 peak 24532 weight 0.10000E+01 volume 0.12534E+01 ppm1 0.843 ppm2 1.613
ASSI {24562}
  (( segid "PROT" and resid 57 and name HG1 ))
  (( segid "PROT" and resid 57 and name HE2 ))
  3.400 2.900 2.100 peak 24562 weight 0.10000E+01 volume 0.70530E+00 ppm1 1.531 ppm2 2.065
ASSI {24592}
  (( segid "PROT" and resid 39 and name HG2 ))
  (( segid "PROT" and resid 43 and name HA ))
  3.400 2.900 2.100 peak 24592 weight 0.10000E+01 volume 0.67070E+00 ppm1 1.463 ppm2 4.989
ASSI {24612}
  (( segid "PROT" and resid 44 and name HG1 ))
  (( segid "PROT" and resid 43 and name HA ))
  3.200 2.600 2.300 peak 24612 weight 0.10000E+01 volume 0.99940E+00 ppm1 2.209 ppm2 4.983
ASSI {24652}
  (( segid "PROT" and resid 32 and name HD1 ))
  (( segid "PROT" and resid 33 and name HD1 ))
  3.600 3.200 1.900 peak 24652 weight 0.10000E+01 volume 0.49260E+00 ppm1 7.899 ppm2 2.263
ASSI {24662}
  (( segid "PROT" and resid 32 and name HD1 ))
  (( segid "PROT" and resid 33 and name HD2 ))
  3.500 3.100 2.000 peak 24662 weight 0.10000E+01 volume 0.59000E+00 ppm1 7.890 ppm2 1.572
ASSI {24692}

```

```

( segid "PROT" and resid 115 and name HD2%)
(( segid "PROT" and resid 113 and name HA ))
3.300 2.700 2.200 peak 24692 weight 0.10000E+01 volume 0.72980E+00 ppm1 0.771 ppm2 4.336
ASSI {24722}
(( segid "PROT" and resid 33 and name HD2 ))
(( segid "PROT" and resid 31 and name HA ))
3.300 2.700 2.200 peak 24722 weight 0.10000E+01 volume 0.77360E+00 ppm1 1.580 ppm2 4.438
ASSI {24732}
(( segid "PROT" and resid 33 and name HD1 ))
(( segid "PROT" and resid 31 and name HA ))
3.200 2.600 2.300 peak 24732 weight 0.10000E+01 volume 0.88700E+00 ppm1 2.262 ppm2 4.438
ASSI {24742}
(( segid "PROT" and resid 34 and name HB2 ))
(( segid "PROT" and resid 31 and name HA ))
3.300 2.700 2.200 peak 24742 weight 0.10000E+01 volume 0.72970E+00 ppm1 2.637 ppm2 4.436
ASSI {24782}
(( segid "PROT" and resid 54 and name HG2 ))
(( segid "PROT" and resid 54 and name HA ))
3.100 2.400 2.400 peak 24782 weight 0.10000E+01 volume 0.11966E+01 ppm1 1.893 ppm2 4.985
ASSI {24792}
(( segid "PROT" and resid 79 and name HG1 ))
(( segid "PROT" and resid 76 and name HA ))
3.300 2.700 2.200 peak 24792 weight 0.10000E+01 volume 0.78020E+00 ppm1 2.452 ppm2 4.113
ASSI {24822}
( segid "PROT" and resid 102 and name HD1%)
(( segid "PROT" and resid 99 and name HA ))
3.200 2.600 2.300 peak 24822 weight 0.10000E+01 volume 0.95780E+00 ppm1 0.759 ppm2 3.907
ASSI {24832}
(( segid "PROT" and resid 102 and name HB2 ))
(( segid "PROT" and resid 99 and name HA ))
3.400 2.900 2.100 peak 24832 weight 0.10000E+01 volume 0.64070E+00 ppm1 1.268 ppm2 3.911
ASSI {24842}
(( segid "PROT" and resid 87 and name HB2 ))
(( segid "PROT" and resid 84 and name HA ))
2.900 2.100 2.100 peak 24842 weight 0.10000E+01 volume 0.16758E+01 ppm1 2.059 ppm2 4.343
ASSI {24852}
( segid "PROT" and resid 82 and name HE%)
(( segid "PROT" and resid 99 and name HA ))
3.400 2.900 2.100 peak 24852 weight 0.10000E+01 volume 0.69880E+00 ppm1 6.487 ppm2 3.907
ASSI {24892}
(( segid "PROT" and resid 10 and name HA ))
(( segid "PROT" and resid 9 and name HA ))
3.200 2.600 2.300 peak 24892 weight 0.10000E+01 volume 0.99840E+00 ppm1 4.935 ppm2 4.357
ASSI {24912}
(( segid "PROT" and resid 56 and name HG ))
(( segid "PROT" and resid 34 and name HA ))
3.500 3.100 2.000 peak 24912 weight 0.10000E+01 volume 0.53580E+00 ppm1 1.755 ppm2 5.006
ASSI {24992}
(( segid "PROT" and resid 30 and name HB1 ))
(( segid "PROT" and resid 102 and name HA ))
3.300 2.700 2.200 peak 24992 weight 0.10000E+01 volume 0.79400E+00 ppm1 4.361 ppm2 3.721
ASSI {25022}
(( segid "PROT" and resid 112 and name HG1 ))
(( segid "PROT" and resid 109 and name HA ))
3.500 3.100 2.000 peak 25022 weight 0.10000E+01 volume 0.52490E+00 ppm1 2.382 ppm2 4.074
ASSI {25032}
(( segid "PROT" and resid 52 and name HA ))
(( segid "PROT" and resid 51 and name HA ))
3.500 3.100 2.000 peak 25032 weight 0.10000E+01 volume 0.59780E+00 ppm1 5.048 ppm2 3.876
ASSI {25092}
(( segid "PROT" and resid 56 and name HB2 ))
(( segid "PROT" and resid 56 and name HA ))
2.400 1.400 1.400 peak 25092 weight 0.10000E+01 volume 0.47870E+01 ppm1 1.422 ppm2 4.075
ASSI {25112}
(( segid "PROT" and resid 21 and name HG11))
(( segid "PROT" and resid 18 and name HA ))
3.300 2.700 2.200 peak 25112 weight 0.10000E+01 volume 0.75700E+00 ppm1 1.776 ppm2 3.313
ASSI {25122}
(( segid "PROT" and resid 21 and name HA ))
(( segid "PROT" and resid 18 and name HA ))
3.300 2.700 2.200 peak 25122 weight 0.10000E+01 volume 0.85990E+00 ppm1 3.800 ppm2 3.313
ASSI {25152}
(( segid "PROT" and resid 73 and name HA ))
(( segid "PROT" and resid 68 and name HA ))
2.900 2.100 2.100 peak 25152 weight 0.10000E+01 volume 0.16472E+01 ppm1 4.267 ppm2 4.561
ASSI {25262}
( segid "PROT" and resid 82 and name HD%)
(( segid "PROT" and resid 103 and name HA ))
3.300 2.700 2.200 peak 25262 weight 0.10000E+01 volume 0.84370E+00 ppm1 6.680 ppm2 3.223
ASSI {25272}
( segid "PROT" and resid 106 and name HD%)
(( segid "PROT" and resid 103 and name HA ))
3.100 2.400 2.400 peak 25272 weight 0.10000E+01 volume 0.12238E+01 ppm1 6.956 ppm2 3.222
ASSI {25312}
(( segid "PROT" and resid 18 and name HB1 ))
(( segid "PROT" and resid 19 and name HA ))
3.500 3.100 2.000 peak 25312 weight 0.10000E+01 volume 0.56690E+00 ppm1 1.567 ppm2 3.719
ASSI {25322}
(( segid "PROT" and resid 109 and name HB2 ))

```

```

(( segid "PROT" and resid 106 and name HA ))
3.300 2.700 2.200 peak 25322 weight 0.10000E+01 volume 0.81090E+00 ppm1 1.582 ppm2 3.997
ASSI {25362}
(( segid "PROT" and resid 77 and name HB1 ))
(( segid "PROT" and resid 74 and name HA ))
3.100 2.400 2.400 peak 25362 weight 0.10000E+01 volume 0.11329E+01 ppm1 2.743 ppm2 3.801
ASSI {25452}
(( segid "PROT" and resid 13 and name HB1 ))
(( segid "PROT" and resid 8 and name HA ))
3.300 2.700 2.200 peak 25452 weight 0.10000E+01 volume 0.83930E+00 ppm1 2.205 ppm2 4.457
ASSI {25462}
(( segid "PROT" and resid 38 and name HA ))
(( segid "PROT" and resid 37 and name HA ))
3.500 3.100 2.000 peak 25462 weight 0.10000E+01 volume 0.51900E+00 ppm1 3.494 ppm2 4.271
ASSI {25512}
(( segid "PROT" and resid 102 and name HD2% ))
(( segid "PROT" and resid 30 and name HB1 ))
3.300 2.700 2.200 peak 25512 weight 0.10000E+01 volume 0.72760E+00 ppm1 0.769 ppm2 4.350
ASSI {25552}
(( segid "PROT" and resid 39 and name HD2 ))
(( segid "PROT" and resid 38 and name HA ))
3.400 2.900 2.100 peak 25552 weight 0.10000E+01 volume 0.70210E+00 ppm1 1.644 ppm2 3.492
ASSI {25612}
(( segid "PROT" and resid 33 and name HD2 ))
(( segid "PROT" and resid 33 and name HA ))
3.400 2.900 2.100 peak 25612 weight 0.10000E+01 volume 0.67050E+00 ppm1 1.563 ppm2 3.990
ASSI {25662}
(( segid "PROT" and resid 18 and name HD2% ))
(( segid "PROT" and resid 17 and name HA ))
3.500 3.100 2.000 peak 25662 weight 0.10000E+01 volume 0.52650E+00 ppm1 -0.159 ppm2 3.972
ASSI {25742}
(( segid "PROT" and resid 18 and name HA ))
(( segid "PROT" and resid 17 and name HB ))
3.300 2.700 2.200 peak 25742 weight 0.10000E+01 volume 0.76330E+00 ppm1 3.321 ppm2 4.267
ASSI {25772}
(( segid "PROT" and resid 33 and name HD1 ))
(( segid "PROT" and resid 31 and name HB% ))
3.100 2.400 2.400 peak 25772 weight 0.10000E+01 volume 0.10817E+01 ppm1 2.264 ppm2 1.762
ASSI {25782}
(( segid "PROT" and resid 34 and name HB2 ))
(( segid "PROT" and resid 31 and name HB% ))
3.600 3.200 1.900 peak 25782 weight 0.10000E+01 volume 0.45500E+00 ppm1 2.622 ppm2 1.754
ASSI {25792}
(( segid "PROT" and resid 25 and name HA ))
(( segid "PROT" and resid 31 and name HB% ))
3.000 2.200 2.200 peak 25792 weight 0.10000E+01 volume 0.14541E+01 ppm1 3.874 ppm2 1.758
ASSI {25802}
(( segid "PROT" and resid 28 and name HA ))
(( segid "PROT" and resid 31 and name HB% ))
3.000 2.200 2.200 peak 25802 weight 0.10000E+01 volume 0.13195E+01 ppm1 4.008 ppm2 1.762
ASSI {25832}
(( segid "PROT" and resid 44 and name HA ))
(( segid "PROT" and resid 43 and name HA ))
3.600 3.200 1.900 peak 25832 weight 0.10000E+01 volume 0.43420E+00 ppm1 4.550 ppm2 4.990
ASSI {25862}
(( segid "PROT" and resid 38 and name HB ))
(( segid "PROT" and resid 43 and name HB% ))
2.400 1.400 1.400 peak 25862 weight 0.10000E+01 volume 0.48630E+01 ppm1 1.079 ppm2 0.972
ASSI {25872}
(( segid "PROT" and resid 39 and name HB2 ))
(( segid "PROT" and resid 43 and name HB% ))
2.400 1.400 1.400 peak 25872 weight 0.10000E+01 volume 0.54502E+01 ppm1 1.924 ppm2 0.978
ASSI {25882}
(( segid "PROT" and resid 44 and name HD2 ))
(( segid "PROT" and resid 43 and name HB% ))
2.900 2.100 2.100 peak 25882 weight 0.10000E+01 volume 0.15646E+01 ppm1 3.567 ppm2 0.988
ASSI {25922}
(( segid "PROT" and resid 102 and name HB1 ))
(( segid "PROT" and resid 99 and name HA ))
3.100 2.400 2.400 peak 25922 weight 0.10000E+01 volume 0.11328E+01 ppm1 1.478 ppm2 3.919
ASSI {25932}
(( segid "PROT" and resid 103 and name HB2 ))
(( segid "PROT" and resid 99 and name HA ))
3.700 3.400 1.800 peak 25932 weight 0.10000E+01 volume 0.39400E+00 ppm1 1.319 ppm2 3.909
ASSI {25942}
(( segid "PROT" and resid 102 and name HG ))
(( segid "PROT" and resid 99 and name HA ))
3.200 2.600 2.300 peak 25942 weight 0.10000E+01 volume 0.89150E+00 ppm1 1.606 ppm2 3.905
ASSI {25962}
(( segid "PROT" and resid 82 and name HB1 ))
(( segid "PROT" and resid 99 and name HA ))
3.700 3.400 1.800 peak 25962 weight 0.10000E+01 volume 0.38960E+00 ppm1 3.153 ppm2 3.915
ASSI {25972}
(( segid "PROT" and resid 98 and name HA ))
(( segid "PROT" and resid 99 and name HA ))
3.400 2.900 2.100 peak 25972 weight 0.10000E+01 volume 0.65570E+00 ppm1 4.227 ppm2 3.919
ASSI {25982}
(( segid "PROT" and resid 34 and name HE% ))
(( segid "PROT" and resid 99 and name HA ))

```

3.500	3.100	2.000	peak 25982	weight	0.10000E+01	volume	0.57510E+00	ppm1	7.199	ppm2	3.918
ASSI {25992}											
((segid "PROT" and resid 86 and name HG1))											
(segid "PROT" and resid 99 and name HB%)											
2.500	1.600	1.600	peak 25992	weight	0.10000E+01	volume	0.45856E+01	ppm1	1.349	ppm2	1.658
ASSI {26002}											
((segid "PROT" and resid 86 and name HB1))											
(segid "PROT" and resid 99 and name HB%)											
2.700	1.800	1.800	peak 26002	weight	0.10000E+01	volume	0.28316E+01	ppm1	1.779	ppm2	1.650
ASSI {26012}											
((segid "PROT" and resid 85 and name HB2))											
(segid "PROT" and resid 99 and name HB%)											
2.400	1.400	1.400	peak 26012	weight	0.10000E+01	volume	0.50444E+01	ppm1	3.088	ppm2	1.657
ASSI {26062}											
(segid "PROT" and resid 17 and name HG2%)											
((segid "PROT" and resid 113 and name HA))											
3.300	2.700	2.200	peak 26062	weight	0.10000E+01	volume	0.74500E+00	ppm1	1.176	ppm2	4.352
ASSI {26072}											
((segid "PROT" and resid 115 and name HG))											
((segid "PROT" and resid 113 and name HA))											
3.600	3.200	1.900	peak 26072	weight	0.10000E+01	volume	0.47150E+00	ppm1	1.567	ppm2	4.354
ASSI {26092}											
((segid "PROT" and resid 112 and name HA))											
((segid "PROT" and resid 113 and name HA))											
3.700	3.400	1.800	peak 26092	weight	0.10000E+01	volume	0.41410E+00	ppm1	4.027	ppm2	4.359
ASSI {26102}											
(segid "PROT" and resid 18 and name HD2%)											
(segid "PROT" and resid 113 and name HB%)											
3.500	3.100	2.000	peak 26102	weight	0.10000E+01	volume	0.53320E+00	ppm1	-0.167	ppm2	1.415
ASSI {26112}											
(segid "PROT" and resid 14 and name HD1%)											
(segid "PROT" and resid 113 and name HB%)											
3.300	2.700	2.200	peak 26112	weight	0.10000E+01	volume	0.78270E+00	ppm1	0.842	ppm2	1.411
ASSI {26122}											
((segid "PROT" and resid 115 and name HB2))											
(segid "PROT" and resid 113 and name HB%)											
2.400	1.400	1.400	peak 26122	weight	0.10000E+01	volume	0.50600E+01	ppm1	1.609	ppm2	1.405
ASSI {26162}											
((segid "PROT" and resid 28 and name HB1))											
((segid "PROT" and resid 25 and name HA))											
3.200	2.600	2.300	peak 26162	weight	0.10000E+01	volume	0.96480E+00	ppm1	3.022	ppm2	3.869
ASSI {26172}											
((segid "PROT" and resid 28 and name HD2))											
((segid "PROT" and resid 25 and name HA))											
3.600	3.200	1.900	peak 26172	weight	0.10000E+01	volume	0.47840E+00	ppm1	5.024	ppm2	3.873
ASSI {26182}											
(segid "PROT" and resid 78 and name HD1%)											
((segid "PROT" and resid 25 and name HB))											
3.600	3.200	1.900	peak 26182	weight	0.10000E+01	volume	0.49810E+00	ppm1	0.104	ppm2	2.445
ASSI {26192}											
(segid "PROT" and resid 102 and name HD2%)											
((segid "PROT" and resid 25 and name HB))											
3.300	2.700	2.200	peak 26192	weight	0.10000E+01	volume	0.72760E+00	ppm1	0.766	ppm2	2.437
ASSI {26202}											
((segid "PROT" and resid 22 and name HA))											
((segid "PROT" and resid 25 and name HB))											
2.500	1.600	1.600	peak 26202	weight	0.10000E+01	volume	0.42061E+01	ppm1	4.151	ppm2	2.441
ASSI {26222}											
(segid "PROT" and resid 63 and name HD1%)											
(segid "PROT" and resid 18 and name HD1%)											
2.800	2.000	2.000	peak 26222	weight	0.10000E+01	volume	0.23014E+01	ppm1	0.880	ppm2	0.513
ASSI {26242}											
((segid "PROT" and resid 85 and name HB1))											
((segid "PROT" and resid 82 and name HA))											
3.200	2.600	2.300	peak 26242	weight	0.10000E+01	volume	0.92110E+00	ppm1	3.421	ppm2	4.230
ASSI {26292}											
(segid "PROT" and resid 102 and name HD2%)											
((segid "PROT" and resid 30 and name HB2))											
3.000	2.200	2.200	peak 26292	weight	0.10000E+01	volume	0.15286E+01	ppm1	0.773	ppm2	3.978
ASSI {26312}											
((segid "PROT" and resid 102 and name HG))											
((segid "PROT" and resid 30 and name HB2))											
3.500	3.100	2.000	peak 26312	weight	0.10000E+01	volume	0.57310E+00	ppm1	1.596	ppm2	3.980
ASSI {26332}											
((segid "PROT" and resid 32 and name HE3))											
((segid "PROT" and resid 32 and name HA))											
3.000	2.200	2.200	peak 26332	weight	0.10000E+01	volume	0.12697E+01	ppm1	7.359	ppm2	4.412
ASSI {26342}											
((segid "PROT" and resid 32 and name HD1))											
((segid "PROT" and resid 32 and name HA))											
3.400	2.900	2.100	peak 26342	weight	0.10000E+01	volume	0.67130E+00	ppm1	7.889	ppm2	4.410
ASSI {26352}											
((segid "PROT" and resid 35 and name HB2))											
((segid "PROT" and resid 32 and name HB1))											
3.500	3.100	2.000	peak 26352	weight	0.10000E+01	volume	0.52260E+00	ppm1	2.213	ppm2	3.637
ASSI {26392}											
((segid "PROT" and resid 32 and name HB2))											
((segid "PROT" and resid 33 and name HD2))											
3.400	2.900	2.100	peak 26392	weight	0.10000E+01	volume	0.60950E+00	ppm1	3.409	ppm2	1.593

```

ASSI {26442}
  ( segid "PROT" and resid 69 and name HG2% )
  ( ( segid "PROT" and resid 11 and name HB1 ) )
  2.800 2.000 2.000 peak 26442 weight 0.10000E+01 volume 0.21371E+01 ppm1 0.863 ppm2 2.357
ASSI {26452}
  ( segid "PROT" and resid 69 and name HG1% )
  ( ( segid "PROT" and resid 11 and name HB1 ) )
  2.800 2.000 2.000 peak 26452 weight 0.10000E+01 volume 0.20188E+01 ppm1 0.990 ppm2 2.356
ASSI {26562}
  ( ( segid "PROT" and resid 54 and name HB2 ) )
  ( ( segid "PROT" and resid 81 and name HA ) )
  3.100 2.400 2.400 peak 26562 weight 0.10000E+01 volume 0.12209E+01 ppm1 1.398 ppm2 3.123
ASSI {26572}
  ( segid "PROT" and resid 73 and name HD1% )
  ( ( segid "PROT" and resid 70 and name HB1 ) )
  3.100 2.400 2.400 peak 26572 weight 0.10000E+01 volume 0.10554E+01 ppm1 0.969 ppm2 4.226
ASSI {26612}
  ( segid "PROT" and resid 68 and name HD% )
  ( ( segid "PROT" and resid 74 and name HA ) )
  2.800 2.000 2.000 peak 26612 weight 0.10000E+01 volume 0.19551E+01 ppm1 7.210 ppm2 3.815
ASSI {26622}
  ( ( segid "PROT" and resid 66 and name HD1 ) )
  ( ( segid "PROT" and resid 67 and name HA ) )
  2.600 1.700 1.700 peak 26622 weight 0.10000E+01 volume 0.32309E+01 ppm1 3.088 ppm2 4.108
ASSI {26632}
  ( segid "PROT" and resid 116 and name HG2% )
  ( ( segid "PROT" and resid 111 and name HA ) )
  2.600 1.700 1.700 peak 26632 weight 0.10000E+01 volume 0.31272E+01 ppm1 0.840 ppm2 4.094
ASSI {26642}
  ( ( segid "PROT" and resid 110 and name HG12 ) )
  ( ( segid "PROT" and resid 111 and name HA ) )
  3.300 2.700 2.200 peak 26642 weight 0.10000E+01 volume 0.86670E+00 ppm1 1.099 ppm2 4.092
ASSI {26692}
  ( ( segid "PROT" and resid 34 and name HZ ) )
  ( segid "PROT" and resid 81 and name HG2% )
  2.700 1.800 1.800 peak 26692 weight 0.10000E+01 volume 0.23973E+01 ppm1 7.278 ppm2 0.151
ASSI {26712}
  ( ( segid "PROT" and resid 82 and name HN ) )
  ( ( segid "PROT" and resid 82 and name HB1 ) )
  3.800 3.600 1.700 peak 26712 weight 0.10000E+01 volume 0.36330E+00 ppm1 6.440 ppm2 3.146
ASSI {26792}
  ( segid "PROT" and resid 107 and name HD% )
  ( ( segid "PROT" and resid 104 and name HA ) )
  3.000 2.200 2.200 peak 26792 weight 0.10000E+01 volume 0.13833E+01 ppm1 7.239 ppm2 4.112
ASSI { 352}
  ( ( segid "PROT" and resid 11 and name HA ) )
  ( ( segid "PROT" and resid 8 and name HG1 ) )
  2.400 2.400 2.100 peak 352 weight 0.10000E+01 volume 0.50737E+01 ppm1 4.376 ppm2 2.024
ASSI { 1382}
  ( ( segid "PROT" and resid 62 and name HA ) )
  ( ( segid "PROT" and resid 65 and name HB2 ) )
  2.800 2.000 2.000 peak 1382 weight 0.10000E+01 volume 0.23053E+01 ppm1 3.907 ppm2 2.808
ASSI { 1392}
  ( ( segid "PROT" and resid 97 and name HA ) )
  ( ( segid "PROT" and resid 92 and name HG2 ) )
  2.600 1.700 1.700 peak 1392 weight 0.10000E+01 volume 0.37031E+01 ppm1 4.250 ppm2 2.295
ASSI { 1442}
  ( ( segid "PROT" and resid 116 and name HA ) )
  ( ( segid "PROT" and resid 6 and name HG1 ) )
  2.700 1.800 1.800 peak 1442 weight 0.10000E+01 volume 0.24084E+01 ppm1 4.257 ppm2 1.453
OR { 1442}
  ( ( segid "PROT" and resid 116 and name HA ) )
  ( ( segid "PROT" and resid 6 and name HG2 ) )
ASSI { 1562}
  ( ( segid "PROT" and resid 103 and name HA ) )
  ( segid "PROT" and resid 82 and name HE% )
  2.800 2.000 2.000 peak 1562 weight 0.10000E+01 volume 0.20471E+01 ppm1 3.221 ppm2 6.482
ASSI { 1622}
  ( ( segid "PROT" and resid 26 and name HA ) )
  ( ( segid "PROT" and resid 26 and name HB1 ) )
  2.300 1.300 1.300 peak 1622 weight 0.10000E+01 volume 0.67915E+01 ppm1 3.934 ppm2 1.916
ASSI { 1662}
  ( ( segid "PROT" and resid 26 and name HA ) )
  ( ( segid "PROT" and resid 26 and name HG1 ) )
  2.700 1.800 1.800 peak 1662 weight 0.10000E+01 volume 0.26801E+01 ppm1 3.935 ppm2 1.533
ASSI { 1912}
  ( ( segid "PROT" and resid 86 and name HA ) )
  ( segid "PROT" and resid 96 and name HE% )
  2.600 1.700 1.700 peak 1912 weight 0.10000E+01 volume 0.36159E+01 ppm1 4.263 ppm2 7.051
ASSI { 3732}
  ( ( segid "PROT" and resid 9 and name HD1 ) )
  ( ( segid "PROT" and resid 7 and name HB1 ) )
  2.900 2.100 2.100 peak 3732 weight 0.10000E+01 volume 0.17407E+01 ppm1 3.222 ppm2 2.070
ASSI { 3742}
  ( ( segid "PROT" and resid 9 and name HD1 ) )
  ( segid "PROT" and resid 14 and name HD1% )
  2.900 2.100 2.100 peak 3742 weight 0.10000E+01 volume 0.15626E+01 ppm1 3.227 ppm2 0.837
OR { 3742}
  ( ( segid "PROT" and resid 9 and name HD1 ) )

```



```

( segid "PROT" and resid 14 and name HD2%)
ASSI { 3962}
(( segid "PROT" and resid 63 and name HB1 ))
(( segid "PROT" and resid 60 and name HB1 ))
2.900 2.100 2.100 peak 3962 weight 0.10000E+01 volume 0.19046E+01 ppm1 2.349 ppm2 4.239
ASSI { 4122}
(( segid "PROT" and resid 6 and name HE1 ))
(( segid "PROT" and resid 116 and name HA ))
2.100 1.100 1.100 peak 4122 weight 0.10000E+01 volume 0.11238E+02 ppm1 3.015 ppm2 4.245
ASSI { 4162}
(( segid "PROT" and resid 64 and name HE1 ))
(( segid "PROT" and resid 61 and name HG1 ))
2.800 2.000 2.000 peak 4162 weight 0.10000E+01 volume 0.19795E+01 ppm1 3.053 ppm2 2.392
ASSI { 4182}
(( segid "PROT" and resid 97 and name HE1 ))
(( segid "PROT" and resid 97 and name HB1 ))
2.300 1.300 1.300 peak 4182 weight 0.10000E+01 volume 0.75764E+01 ppm1 3.027 ppm2 2.101
ASSI { 4222}
(( segid "PROT" and resid 19 and name HE1 ))
(( segid "PROT" and resid 19 and name HG1 ))
2.200 1.200 1.200 peak 4222 weight 0.10000E+01 volume 0.87095E+01 ppm1 2.967 ppm2 1.310
ASSI { 4252}
(( segid "PROT" and resid 19 and name HE1 ))
( segid "PROT" and resid 63 and name HD1%)
2.800 2.000 2.000 peak 4252 weight 0.10000E+01 volume 0.20298E+01 ppm1 2.990 ppm2 0.921
ASSI { 4612}
(( segid "PROT" and resid 86 and name HE1 ))
(( segid "PROT" and resid 103 and name HB1 ))
2.800 2.000 2.000 peak 4612 weight 0.10000E+01 volume 0.21144E+01 ppm1 2.508 ppm2 1.828
ASSI { 4632}
(( segid "PROT" and resid 86 and name HE1 ))
( segid "PROT" and resid 99 and name HB%)
2.800 2.000 2.000 peak 4632 weight 0.10000E+01 volume 0.19300E+01 ppm1 2.506 ppm2 1.665
ASSI { 4672}
(( segid "PROT" and resid 86 and name HE1 ))
(( segid "PROT" and resid 86 and name HD1 ))
2.400 1.400 1.400 peak 4672 weight 0.10000E+01 volume 0.59325E+01 ppm1 2.506 ppm2 1.340
OR { 4672}
(( segid "PROT" and resid 86 and name HE1 ))
(( segid "PROT" and resid 86 and name HG1 ))
ASSI { 4742}
(( segid "PROT" and resid 86 and name HE1 ))
(( segid "PROT" and resid 86 and name HG2 ))
2.900 2.100 2.100 peak 4742 weight 0.10000E+01 volume 0.16989E+01 ppm1 2.498 ppm2 0.168
OR { 4742}
(( segid "PROT" and resid 86 and name HE2 ))
(( segid "PROT" and resid 86 and name HG2 ))
ASSI { 6012}
(( segid "PROT" and resid 42 and name HG2 ))
(( segid "PROT" and resid 39 and name HG1 ))
2.700 1.800 1.800 peak 6012 weight 0.10000E+01 volume 0.29022E+01 ppm1 2.303 ppm2 1.675
ASSI { 6632}
(( segid "PROT" and resid 111 and name HB1 ))
(( segid "PROT" and resid 111 and name HD1 ))
1.900 0.900 0.900 peak 6632 weight 0.10000E+01 volume 0.19710E+02 ppm1 1.940 ppm2 1.692
ASSI { 6682}
(( segid "PROT" and resid 86 and name HB1 ))
( segid "PROT" and resid 96 and name HE%)
2.900 2.100 2.100 peak 6682 weight 0.10000E+01 volume 0.16294E+01 ppm1 1.808 ppm2 7.051
ASSI { 6922}
(( segid "PROT" and resid 64 and name HB1 ))
(( segid "PROT" and resid 61 and name HA ))
2.200 1.200 1.200 peak 6922 weight 0.10000E+01 volume 0.80769E+01 ppm1 2.068 ppm2 4.094
ASSI { 7882}
(( segid "PROT" and resid 86 and name HD1 ))
( segid "PROT" and resid 96 and name HE%)
3.000 2.200 2.200 peak 7882 weight 0.10000E+01 volume 0.15219E+01 ppm1 1.364 ppm2 7.049
ASSI { 7892}
(( segid "PROT" and resid 19 and name HD1 ))
( segid "PROT" and resid 15 and name HE%)
2.600 1.700 1.700 peak 7892 weight 0.10000E+01 volume 0.34592E+01 ppm1 1.640 ppm2 6.922
ASSI { 7922}
(( segid "PROT" and resid 86 and name HD1 ))
(( segid "PROT" and resid 86 and name HA ))
2.900 2.100 2.100 peak 7922 weight 0.10000E+01 volume 0.18440E+01 ppm1 1.341 ppm2 4.265
ASSI { 7952}
(( segid "PROT" and resid 112 and name HB1 ))
(( segid "PROT" and resid 109 and name HA ))
2.100 1.100 1.100 peak 7952 weight 0.10000E+01 volume 0.11736E+02 ppm1 2.106 ppm2 4.081
ASSI { 7982}
(( segid "PROT" and resid 57 and name HD1 ))
(( segid "PROT" and resid 37 and name HD1 ))
2.700 1.800 1.800 peak 7982 weight 0.10000E+01 volume 0.28210E+01 ppm1 1.730 ppm2 3.708
ASSI { 8012}
(( segid "PROT" and resid 86 and name HD1 ))
(( segid "PROT" and resid 86 and name HE1 ))
2.700 1.800 1.800 peak 8012 weight 0.10000E+01 volume 0.27789E+01 ppm1 1.336 ppm2 2.524
ASSI { 8032}
(( segid "PROT" and resid 86 and name HD1 ))

```

```

    (( segid "PROT" and resid 86 and name HE2 ))
    2.600 1.700 1.700 peak 8032 weight 0.10000E+01 volume 0.29928E+01 ppm1 1.368 ppm2 2.471
OR { 8032}
    (( segid "PROT" and resid 86 and name HD1 ))
    (( segid "PROT" and resid 86 and name HE1 ))
ASSI { 8072}
    (( segid "PROT" and resid 111 and name HD1 ))
    (( segid "PROT" and resid 112 and name HG2 ))
    2.400 2.400 2.100 peak 8072 weight 0.10000E+01 volume 0.48306E+01 ppm1 1.696 ppm2 2.215
ASSI { 8102}
    (( segid "PROT" and resid 86 and name HD1 ))
    (( segid "PROT" and resid 86 and name HG2 ))
    2.400 1.400 1.400 peak 8102 weight 0.10000E+01 volume 0.47467E+01 ppm1 1.360 ppm2 0.169
ASSI { 8182}
    (( segid "PROT" and resid 64 and name HD1 ))
    (( segid "PROT" and resid 64 and name HB1 ))
    2.000 1.000 1.000 peak 8182 weight 0.10000E+01 volume 0.14643E+02 ppm1 1.792 ppm2 2.096
ASSI { 8242}
    (( segid "PROT" and resid 39 and name HD2 ))
    (( segid "PROT" and resid 39 and name HA ))
    2.600 1.700 1.700 peak 8242 weight 0.10000E+01 volume 0.30605E+01 ppm1 1.676 ppm2 4.452
ASSI { 8742}
    (( segid "PROT" and resid 78 and name HG ))
    (( segid "PROT" and resid 82 and name HE% ))
    3.000 2.200 2.200 peak 8742 weight 0.10000E+01 volume 0.15179E+01 ppm1 0.689 ppm2 6.468
ASSI { 9112}
    (( segid "PROT" and resid 115 and name HG ))
    (( segid "PROT" and resid 75 and name HG2 ))
    2.900 2.100 2.100 peak 9112 weight 0.10000E+01 volume 0.18866E+01 ppm1 1.545 ppm2 2.216
ASSI { 9162}
    (( segid "PROT" and resid 56 and name HG ))
    (( segid "PROT" and resid 56 and name HE2 ))
    2.800 2.000 2.000 peak 9162 weight 0.10000E+01 volume 0.19931E+01 ppm1 1.776 ppm2 1.409
ASSI { 9412}
    (( segid "PROT" and resid 26 and name HG1 ))
    (( segid "PROT" and resid 26 and name HB1 ))
    2.100 1.100 1.100 peak 9412 weight 0.10000E+01 volume 0.12118E+02 ppm1 1.528 ppm2 1.896
ASSI { 9452}
    (( segid "PROT" and resid 63 and name HG ))
    (( segid "PROT" and resid 18 and name HB1 ))
    2.300 1.300 1.300 peak 9452 weight 0.10000E+01 volume 0.69171E+01 ppm1 1.875 ppm2 1.539
ASSI { 9522}
    (( segid "PROT" and resid 26 and name HG1 ))
    (( segid "PROT" and resid 56 and name HD1% ))
    2.600 1.700 1.700 peak 9522 weight 0.10000E+01 volume 0.30036E+01 ppm1 1.532 ppm2 0.976
ASSI { 9982}
    (( segid "PROT" and resid 97 and name HG1 ))
    (( segid "PROT" and resid 97 and name HE1 ))
    2.600 1.700 1.700 peak 9982 weight 0.10000E+01 volume 0.35375E+01 ppm1 1.844 ppm2 3.009
ASSI {10022}
    (( segid "PROT" and resid 97 and name HG2 ))
    (( segid "PROT" and resid 97 and name HG1 ))
    2.000 1.000 1.000 peak 10022 weight 0.10000E+01 volume 0.17308E+02 ppm1 1.609 ppm2 1.842
ASSI {10202}
    (( segid "PROT" and resid 39 and name HG1 ))
    (( segid "PROT" and resid 39 and name HA ))
    2.700 1.800 1.800 peak 10202 weight 0.10000E+01 volume 0.28740E+01 ppm1 1.623 ppm2 4.451
ASSI {10212}
    (( segid "PROT" and resid 39 and name HG2 ))
    (( segid "PROT" and resid 39 and name HA ))
    2.500 1.600 1.600 peak 10212 weight 0.10000E+01 volume 0.46613E+01 ppm1 1.470 ppm2 4.449
ASSI {10612}
    (( segid "PROT" and resid 102 and name HD1% ))
    (( segid "PROT" and resid 34 and name HZ ))
    2.500 1.600 1.600 peak 10612 weight 0.10000E+01 volume 0.42774E+01 ppm1 0.762 ppm2 7.257
ASSI {10622}
    (( segid "PROT" and resid 102 and name HD1% ))
    (( segid "PROT" and resid 34 and name HD% ))
    2.500 1.600 1.600 peak 10622 weight 0.10000E+01 volume 0.45270E+01 ppm1 0.763 ppm2 7.189
OR {10622}
    (( segid "PROT" and resid 102 and name HD1% ))
    (( segid "PROT" and resid 34 and name HE% ))
ASSI {10642}
    (( segid "PROT" and resid 57 and name HG1 ))
    (( segid "PROT" and resid 37 and name HA ))
    2.400 1.400 1.400 peak 10642 weight 0.10000E+01 volume 0.51970E+01 ppm1 1.545 ppm2 4.249
ASSI {10822}
    (( segid "PROT" and resid 64 and name HG1 ))
    (( segid "PROT" and resid 64 and name HB1 ))
    2.100 1.100 1.100 peak 10822 weight 0.10000E+01 volume 0.11069E+02 ppm1 1.647 ppm2 2.091
ASSI {10832}
    (( segid "PROT" and resid 6 and name HC1 ))
    (( segid "PROT" and resid 6 and name HB1 ))
    2.000 1.000 1.000 peak 10832 weight 0.10000E+01 volume 0.14254E+02 ppm1 1.459 ppm2 1.889
OR {10832}
    (( segid "PROT" and resid 6 and name HG2 ))
    (( segid "PROT" and resid 6 and name HB1 ))
ASSI {10842}
    (( segid "PROT" and resid 64 and name HG1 ))

```

```

(( segid "PROT" and resid 64 and name HD1 ))
1.900 0.900 0.900 peak 10842 weight 0.10000E+01 volume 0.24855E+02 ppm1 1.623 ppm2 1.783
ASSI {10892}
(( segid "PROT" and resid 19 and name HG1 ))
(( segid "PROT" and resid 63 and name HD1 ))
2.400 1.400 1.400 peak 10892 weight 0.10000E+01 volume 0.52665E+01 ppm1 1.302 ppm2 0.919
ASSI {11172}
(( segid "PROT" and resid 22 and name HD2 ))
(( segid "PROT" and resid 74 and name HE ))
2.400 2.400 2.100 peak 11172 weight 0.10000E+01 volume 0.54920E+01 ppm1 1.050 ppm2 6.962
ASSI {11252}
(( segid "PROT" and resid 22 and name HD2 ))
(( segid "PROT" and resid 25 and name HG1 ))
2.600 1.700 1.700 peak 11252 weight 0.10000E+01 volume 0.33026E+01 ppm1 1.054 ppm2 1.253
ASSI {11392}
(( segid "PROT" and resid 109 and name HG1 ))
(( segid "PROT" and resid 109 and name HB1 ))
2.200 1.200 1.200 peak 11392 weight 0.10000E+01 volume 0.98792E+01 ppm1 0.815 ppm2 1.750
ASSI {11712}
(( segid "PROT" and resid 38 and name HG1 ))
(( segid "PROT" and resid 46 and name HE ))
2.600 1.700 1.700 peak 11712 weight 0.10000E+01 volume 0.34807E+01 ppm1 0.496 ppm2 5.996
ASSI {11822}
(( segid "PROT" and resid 41 and name HG2 ))
(( segid "PROT" and resid 42 and name HG2 ))
2.800 2.000 2.000 peak 11822 weight 0.10000E+01 volume 0.20436E+01 ppm1 1.342 ppm2 2.237
OR {11822}
(( segid "PROT" and resid 41 and name HG2 ))
(( segid "PROT" and resid 42 and name HB1 ))
ASSI {12062}
(( segid "PROT" and resid 81 and name HG2 ))
(( segid "PROT" and resid 56 and name HG ))
2.800 2.000 2.000 peak 12062 weight 0.10000E+01 volume 0.19114E+01 ppm1 0.159 ppm2 1.772
ASSI {12272}
(( segid "PROT" and resid 49 and name HG2 ))
(( segid "PROT" and resid 88 and name HD ))
2.600 1.700 1.700 peak 12272 weight 0.10000E+01 volume 0.34730E+01 ppm1 0.946 ppm2 6.976
ASSI {12392}
(( segid "PROT" and resid 18 and name HD2 ))
(( segid "PROT" and resid 74 and name HE ))
2.700 1.800 1.800 peak 12392 weight 0.10000E+01 volume 0.28804E+01 ppm1 -0.158 ppm2 6.969
ASSI {12842}
(( segid "PROT" and resid 110 and name HG2 ))
(( segid "PROT" and resid 21 and name HG2 ))
2.400 1.400 1.400 peak 12842 weight 0.10000E+01 volume 0.57140E+01 ppm1 0.693 ppm2 1.023
ASSI {13192}
(( segid "PROT" and resid 21 and name HG2 ))
(( segid "PROT" and resid 110 and name HD1 ))
2.800 2.000 2.000 peak 13192 weight 0.10000E+01 volume 0.20914E+01 ppm1 1.018 ppm2 0.571
ASSI {13312}
(( segid "PROT" and resid 75 and name HE ))
(( segid "PROT" and resid 79 and name HB1 ))
2.800 2.000 2.000 peak 13312 weight 0.10000E+01 volume 0.21237E+01 ppm1 2.092 ppm2 2.493
ASSI {13522}
(( segid "PROT" and resid 59 and name HE ))
(( segid "PROT" and resid 74 and name HE ))
2.500 1.600 1.600 peak 13522 weight 0.10000E+01 volume 0.46777E+01 ppm1 1.309 ppm2 6.967
ASSI {13532}
(( segid "PROT" and resid 59 and name HE ))
(( segid "PROT" and resid 74 and name HD ))
2.800 2.000 2.000 peak 13532 weight 0.10000E+01 volume 0.22023E+01 ppm1 1.313 ppm2 6.438
ASSI {13882}
(( segid "PROT" and resid 101 and name HD1 ))
(( segid "PROT" and resid 97 and name HB1 ))
3.000 2.200 2.200 peak 13882 weight 0.10000E+01 volume 0.15141E+01 ppm1 0.992 ppm2 3.007
ASSI {14042}
(( segid "PROT" and resid 116 and name HD1 ))
(( segid "PROT" and resid 75 and name HB1 ))
2.900 2.100 2.100 peak 14042 weight 0.10000E+01 volume 0.17704E+01 ppm1 0.827 ppm2 2.933
ASSI {14122}
(( segid "PROT" and resid 116 and name HD1 ))
(( segid "PROT" and resid 110 and name HG12 ))
2.600 1.700 1.700 peak 14122 weight 0.10000E+01 volume 0.30126E+01 ppm1 0.821 ppm2 1.083
ASSI {14172}
(( segid "PROT" and resid 110 and name HD1 ))
(( segid "PROT" and resid 107 and name HD ))
2.700 1.800 1.800 peak 14172 weight 0.10000E+01 volume 0.25688E+01 ppm1 0.568 ppm2 7.237
ASSI {14532}
(( segid "PROT" and resid 17 and name HG2 ))
(( segid "PROT" and resid 18 and name HD1 ))
3.100 2.400 2.400 peak 14532 weight 0.10000E+01 volume 0.11123E+01 ppm1 1.184 ppm2 0.520
ASSI {15272}
(( segid "PROT" and resid 81 and name HG1 ))
(( segid "PROT" and resid 34 and name HD ))
3.200 2.600 2.300 peak 15272 weight 0.10000E+01 volume 0.91000E+00 ppm1 0.499 ppm2 7.183
OR {15272}
(( segid "PROT" and resid 81 and name HG1 ))
(( segid "PROT" and resid 34 and name HE ))
ASSI {15312}

```

```

( segid "PROT" and resid 38 and name HG2%)
( segid "PROT" and resid 46 and name HE%)
3.000 2.200 2.200 peak 15312 weight 0.10000E+01 volume 0.14457E+01 ppm1 -0.010 ppm2 5.996
ASSI {15362}
( segid "PROT" and resid 38 and name HG2%)
(( segid "PROT" and resid 46 and name HB1 ))
3.100 2.400 2.400 peak 15362 weight 0.10000E+01 volume 0.10649E+01 ppm1 -0.007 ppm2 2.757
ASSI {15892}
( segid "PROT" and resid 56 and name HD2%)
( segid "PROT" and resid 25 and name HG1%)
3.100 2.400 2.400 peak 15892 weight 0.10000E+01 volume 0.10650E+01 ppm1 0.679 ppm2 1.248
ASSI {16042}
(( segid "PROT" and resid 63 and name HB2 ))
(( segid "PROT" and resid 60 and name HB1 ))
3.200 2.600 2.300 peak 16042 weight 0.10000E+01 volume 0.96490E+00 ppm1 1.967 ppm2 4.248
ASSI {16132}
( segid "PROT" and resid 63 and name HD2%)
( segid "PROT" and resid 74 and name HD%)
3.100 2.400 2.400 peak 16132 weight 0.10000E+01 volume 0.11722E+01 ppm1 1.080 ppm2 6.426
ASSI {16252}
( segid "PROT" and resid 73 and name HD2%)
(( segid "PROT" and resid 70 and name HB2 ))
3.200 2.600 2.300 peak 16252 weight 0.10000E+01 volume 0.96550E+00 ppm1 0.929 ppm2 3.790
ASSI {16922}
( segid "PROT" and resid 50 and name HD1%)
( segid "PROT" and resid 88 and name HD%)
3.000 2.200 2.200 peak 16922 weight 0.10000E+01 volume 0.13378E+01 ppm1 0.582 ppm2 6.971
ASSI {17102}
( segid "PROT" and resid 101 and name HG2%)
(( segid "PROT" and resid 29 and name HB1 ))
3.400 2.900 2.100 peak 17102 weight 0.10000E+01 volume 0.61290E+00 ppm1 1.029 ppm2 2.109
ASSI {17302}
(( segid "PROT" and resid 116 and name HB ))
( segid "PROT" and resid 110 and name HG2%)
3.300 2.700 2.200 peak 17302 weight 0.10000E+01 volume 0.80280E+00 ppm1 1.852 ppm2 0.694
ASSI {18462}
(( segid "PROT" and resid 54 and name HB1 ))
( segid "PROT" and resid 58 and name HG2%)
3.400 2.900 2.100 peak 18462 weight 0.10000E+01 volume 0.64170E+00 ppm1 2.058 ppm2 1.120
ASSI {18482}
( segid "PROT" and resid 59 and name HE%)
( segid "PROT" and resid 18 and name HD2%)
3.400 2.900 2.100 peak 18482 weight 0.10000E+01 volume 0.60840E+00 ppm1 1.306 ppm2 -0.172
ASSI {18852}
(( segid "PROT" and resid 64 and name HA ))
(( segid "PROT" and resid 64 and name HB1 ))
2.100 1.100 1.100 peak 18852 weight 0.10000E+01 volume 0.11301E+02 ppm1 4.374 ppm2 2.092
ASSI {19072}
(( segid "PROT" and resid 45 and name HA1 ))
(( segid "PROT" and resid 44 and name HA ))
3.300 2.700 2.200 peak 19072 weight 0.10000E+01 volume 0.78950E+00 ppm1 3.907 ppm2 4.526
ASSI {19292}
(( segid "PROT" and resid 97 and name HG1 ))
( segid "PROT" and resid 97 and name HB1 ))
2.200 1.200 1.200 peak 19292 weight 0.10000E+01 volume 0.81546E+01 ppm1 1.853 ppm2 2.117
ASSI {19312}
(( segid "PROT" and resid 97 and name HG2 ))
(( segid "PROT" and resid 97 and name HB1 ))
2.300 1.300 1.300 peak 19312 weight 0.10000E+01 volume 0.65967E+01 ppm1 1.608 ppm2 2.109
ASSI {19392}
( segid "PROT" and resid 49 and name HG1%)
(( segid "PEPT" and resid 202 and name HB1 ))
2.700 1.800 1.800 peak 19392 weight 0.10000E+01 volume 0.25893E+01 ppm1 0.974 ppm2 3.133
ASSI {19542}
(( segid "PROT" and resid 53 and name HD2 ))
(( segid "PROT" and resid 51 and name HB2 ))
3.500 3.100 2.000 peak 19542 weight 0.10000E+01 volume 0.55650E+00 ppm1 3.438 ppm2 1.208
OR {19542}
(( segid "PROT" and resid 53 and name HD2 ))
(( segid "PROT" and resid 51 and name HG2 ))
ASSI {19902}
( segid "PROT" and resid 49 and name HG2%)
( segid "PEPT" and resid 202 and name HD%)
2.800 2.000 2.000 peak 19902 weight 0.10000E+01 volume 0.19805E+01 ppm1 0.950 ppm2 7.165
ASSI {20122}
(( segid "PROT" and resid 36 and name HB1 ))
(( segid "PROT" and resid 37 and name HD1 ))
2.500 1.600 1.600 peak 20122 weight 0.10000E+01 volume 0.43249E+01 ppm1 2.155 ppm2 3.703
ASSI {20352}
(( segid "PROT" and resid 82 and name HB2 ))
( segid "PROT" and resid 82 and name HE%)
3.500 3.100 2.000 peak 20352 weight 0.10000E+01 volume 0.57940E+00 ppm1 3.014 ppm2 6.489
ASSI {20372}
(( segid "PROT" and resid 106 and name HB1 ))
( segid "PROT" and resid 82 and name HE%)
3.100 2.400 2.400 peak 20372 weight 0.10000E+01 volume 0.12466E+01 ppm1 3.360 ppm2 6.464
ASSI {20402}
(( segid "PROT" and resid 106 and name HA ))
( segid "PROT" and resid 110 and name HG2%)

```

```

3.500    3.100    2.000 peak 20402 weight 0.10000E+01 volume 0.59050E+00 ppm1 4.003 ppm2 0.702
ASSI {20782}
( segid "PROT" and resid 38 and name HG2% )
(( segid "PROT" and resid 39 and name HG2 ))
3.300    2.700    2.200 peak 20782 weight 0.10000E+01 volume 0.72730E+00 ppm1 -0.003 ppm2 1.478
ASSI {20982}
(( segid "PROT" and resid 26 and name HG1 ))
(( segid "PROT" and resid 35 and name HG1 ))
3.200    2.600    2.300 peak 20982 weight 0.10000E+01 volume 0.10083E+01 ppm1 1.534 ppm2 2.892
ASSI {21042}
( segid "PROT" and resid 50 and name HD1% )
( segid "PROT" and resid 88 and name HE% )
3.300    2.700    2.200 peak 21042 weight 0.10000E+01 volume 0.73200E+00 ppm1 0.582 ppm2 6.661
ASSI {21132}
( segid "PROT" and resid 116 and name HD1% )
( segid "PROT" and resid 107 and name HD% )
3.000    2.200    2.200 peak 21132 weight 0.10000E+01 volume 0.14426E+01 ppm1 0.827 ppm2 7.236
ASSI {21212}
( segid "PROT" and resid 21 and name HD1% )
(( segid "PROT" and resid 74 and name HB1 ))
3.200    2.600    2.300 peak 21212 weight 0.10000E+01 volume 0.96830E+00 ppm1 0.656 ppm2 3.041
ASSI {21232}
( segid "PROT" and resid 21 and name HD1% )
(( segid "PROT" and resid 17 and name HB ))
3.100    2.400    2.400 peak 21232 weight 0.10000E+01 volume 0.11130E+01 ppm1 0.652 ppm2 4.288
ASSI {21342}
( segid "PROT" and resid 35 and name HE% )
(( segid "PROT" and resid 32 and name HH2 ))
3.500    3.100    2.000 peak 21342 weight 0.10000E+01 volume 0.55660E+00 ppm1 2.216 ppm2 7.208
ASSI {21352}
( segid "PROT" and resid 75 and name HE% )
( segid "PROT" and resid 78 and name HD1% )
3.500    3.100    2.000 peak 21352 weight 0.10000E+01 volume 0.57510E+00 ppm1 2.099 ppm2 0.091
ASSI {21362}
( segid "PROT" and resid 75 and name HE% )
( segid "PROT" and resid 21 and name HG2% )
3.500    3.100    2.000 peak 21362 weight 0.10000E+01 volume 0.58360E+00 ppm1 2.096 ppm2 1.033
ASSI {21372}
( segid "PROT" and resid 75 and name HE% )
(( segid "PROT" and resid 110 and name HG12 ))
3.400    2.900    2.100 peak 21372 weight 0.10000E+01 volume 0.62060E+00 ppm1 2.096 ppm2 1.085
ASSI {21412}
( segid "PROT" and resid 75 and name HE% )
( segid "PROT" and resid 74 and name HD% )
3.700    3.400    1.800 peak 21412 weight 0.10000E+01 volume 0.41590E+00 ppm1 2.095 ppm2 6.444
ASSI {21452}
( segid "PROT" and resid 21 and name HG2% )
( segid "PROT" and resid 74 and name HD% )
3.400    2.900    2.100 peak 21452 weight 0.10000E+01 volume 0.69490E+00 ppm1 1.011 ppm2 6.431
ASSI {21502}
( segid "PROT" and resid 101 and name HG2% )
( segid "PROT" and resid 102 and name HD2% )
2.500    1.600    1.600 peak 21502 weight 0.10000E+01 volume 0.44117E+01 ppm1 1.031 ppm2 0.764
OR {21502}
( segid "PROT" and resid 101 and name HG2% )
( segid "PROT" and resid 102 and name HD1% )
ASSI {21572}
( segid "PROT" and resid 116 and name HG2% )
(( segid "PROT" and resid 117 and name HA ))
3.400    2.900    2.100 peak 21572 weight 0.10000E+01 volume 0.69010E+00 ppm1 0.856 ppm2 4.600
ASSI {21612}
( segid "PROT" and resid 99 and name HB% )
(( segid "PROT" and resid 33 and name HG2 ))
3.700    3.400    1.800 peak 21612 weight 0.10000E+01 volume 0.42110E+00 ppm1 1.661 ppm2 -0.880
ASSI {21642}
( segid "PROT" and resid 76 and name HB% )
(( segid "PROT" and resid 72 and name HD1 ))
2.300    2.300    2.200 peak 21642 weight 0.10000E+01 volume 0.65500E+01 ppm1 1.523 ppm2 1.658
ASSI {21742}
( segid "PROT" and resid 99 and name HB% )
(( segid "PROT" and resid 85 and name HA ))
3.400    2.900    2.100 peak 21742 weight 0.10000E+01 volume 0.65540E+00 ppm1 1.659 ppm2 4.510
ASSI {21812}
( segid "PROT" and resid 110 and name HG2% )
( segid "PROT" and resid 113 and name HB% )
2.900    2.100    2.100 peak 21812 weight 0.10000E+01 volume 0.18327E+01 ppm1 0.692 ppm2 1.411
ASSI {21822}
( segid "PROT" and resid 69 and name HG2% )
(( segid "PROT" and resid 14 and name HB1 ))
3.100    2.400    2.400 peak 21822 weight 0.10000E+01 volume 0.12228E+01 ppm1 0.861 ppm2 1.850
ASSI {21832}
( segid "PROT" and resid 69 and name HG2% )
(( segid "PROT" and resid 68 and name HA ))
3.400    2.900    2.100 peak 21832 weight 0.10000E+01 volume 0.62230E+00 ppm1 0.861 ppm2 4.575
ASSI {21872}
( segid "PROT" and resid 113 and name HB% )
( segid "PROT" and resid 110 and name HD1% )
3.000    2.200    2.200 peak 21872 weight 0.10000E+01 volume 0.12843E+01 ppm1 1.412 ppm2 0.572
ASSI {21902}

```

```

( segid "PROT" and resid 113 and name HB% )
(( segid "PROT" and resid 17 and name HA ))
3.000 2.200 2.200 peak 21902 weight 0.10000E+01 volume 0.13747E+01 ppm1 1.409 ppm2 3.966
ASSI {22082}
( segid "PROT" and resid 81 and name HG2% )
(( segid "PROT" and resid 55 and name HB1 ))
3.600 3.200 1.900 peak 22082 weight 0.10000E+01 volume 0.43360E+00 ppm1 0.155 ppm2 2.405
ASSI {22182}
( segid "PROT" and resid 56 and name HD2% )
(( segid "PROT" and resid 78 and name HA ))
3.400 2.900 2.100 peak 22182 weight 0.10000E+01 volume 0.66210E+00 ppm1 0.675 ppm2 3.414
ASSI {22202}
( segid "PROT" and resid 56 and name HD2% )
( segid "PROT" and resid 34 and name HD% )
3.500 3.100 2.000 peak 22202 weight 0.10000E+01 volume 0.59280E+00 ppm1 0.675 ppm2 7.196
OR {22202}
( segid "PROT" and resid 56 and name HD2% )
( segid "PROT" and resid 34 and name HE% )
ASSI {22212}
( segid "PROT" and resid 25 and name HG1% )
( segid "PROT" and resid 82 and name HE% )
3.200 2.600 2.300 peak 22212 weight 0.10000E+01 volume 0.89620E+00 ppm1 1.241 ppm2 6.454
ASSI {22352}
( segid "PROT" and resid 22 and name HD2% )
( segid "PROT" and resid 74 and name HD% )
3.300 2.700 2.200 peak 22352 weight 0.10000E+01 volume 0.78330E+00 ppm1 1.052 ppm2 6.445
ASSI {22472}
( segid "PROT" and resid 102 and name HD2% )
(( segid "PROT" and resid 31 and name HA ))
2.600 1.700 1.700 peak 22472 weight 0.10000E+01 volume 0.31247E+01 ppm1 0.765 ppm2 4.437
ASSI {22502}
( segid "PROT" and resid 78 and name HD2% )
( segid "PROT" and resid 82 and name HD% )
3.300 2.700 2.200 peak 22502 weight 0.10000E+01 volume 0.80400E+00 ppm1 0.199 ppm2 6.702
ASSI {22602}
( segid "PROT" and resid 102 and name HD1% )
( segid "PROT" and resid 82 and name HD% )
3.500 3.100 2.000 peak 22602 weight 0.10000E+01 volume 0.58490E+00 ppm1 0.762 ppm2 6.676
ASSI {22622}
(( segid "PROT" and resid 57 and name HG1 ))
(( segid "PROT" and resid 57 and name HD2 ))
3.100 2.400 2.400 peak 22622 weight 0.10000E+01 volume 0.12324E+01 ppm1 1.569 ppm2 0.932
ASSI {22632}
(( segid "PROT" and resid 111 and name HG1 ))
(( segid "PROT" and resid 116 and name HG12 ))
3.200 2.600 2.300 peak 22632 weight 0.10000E+01 volume 0.10190E+01 ppm1 1.464 ppm2 0.938
ASSI {22672}
( segid "PROT" and resid 115 and name HD1% )
(( segid "PROT" and resid 75 and name HG2 ))
3.200 2.600 2.300 peak 22672 weight 0.10000E+01 volume 0.10174E+01 ppm1 0.744 ppm2 2.225
ASSI {22782}
(( segid "PROT" and resid 33 and name HG1 ))
( segid "PROT" and resid 95 and name HD% )
3.400 2.900 2.100 peak 22782 weight 0.10000E+01 volume 0.69740E+00 ppm1 0.267 ppm2 6.866
ASSI {22812}
( segid "PROT" and resid 73 and name HD1% )
(( segid "PROT" and resid 69 and name HB ))
3.100 2.400 2.400 peak 22812 weight 0.10000E+01 volume 0.12027E+01 ppm1 0.970 ppm2 2.351
ASSI {22872}
( segid "PROT" and resid 78 and name HD1% )
(( segid "PROT" and resid 106 and name HA ))
3.100 2.400 2.400 peak 22872 weight 0.10000E+01 volume 0.10589E+01 ppm1 0.094 ppm2 3.962
ASSI {22882}
( segid "PROT" and resid 78 and name HD1% )
(( segid "PROT" and resid 22 and name HA ))
3.300 2.700 2.200 peak 22882 weight 0.10000E+01 volume 0.75140E+00 ppm1 0.089 ppm2 4.153
ASSI {22922}
( segid "PROT" and resid 22 and name HD1% )
(( segid "PROT" and resid 63 and name HB1 ))
3.000 2.200 2.200 peak 22922 weight 0.10000E+01 volume 0.14674E+01 ppm1 1.109 ppm2 2.349
ASSI {23192}
(( segid "PROT" and resid 66 and name HG2 ))
(( segid "PROT" and resid 69 and name HB ))
3.500 3.100 2.000 peak 23192 weight 0.10000E+01 volume 0.59710E+00 ppm1 1.566 ppm2 2.327
ASSI {23212}
(( segid "PROT" and resid 53 and name HG1 ))
( segid "PROT" and resid 46 and name HE% )
3.200 2.600 2.300 peak 23212 weight 0.10000E+01 volume 0.94430E+00 ppm1 2.282 ppm2 5.997
ASSI {23222}
(( segid "PROT" and resid 53 and name HG2 ))
( segid "PROT" and resid 46 and name HE% )
3.200 2.600 2.300 peak 23222 weight 0.10000E+01 volume 0.88660E+00 ppm1 1.933 ppm2 5.988
ASSI {23392}
(( segid "PROT" and resid 87 and name HB1 ))
( segid "PROT" and resid 83 and name HG2% )
3.400 2.900 2.100 peak 23392 weight 0.10000E+01 volume 0.68860E+00 ppm1 2.232 ppm2 1.344
ASSI {23482}
(( segid "PROT" and resid 54 and name HB2 ))
(( segid "PROT" and resid 80 and name HG1 ))

```

```

3.000      2.200      2.200 peak 23482 weight 0.10000E+01 volume 0.12929E+01 ppm1 1.385 ppm2 1.761
ASSI {23502}
(( segid "PROT" and resid 86 and name HB1 ))
(( segid "PROT" and resid 86 and name HG2 ))
3.000      2.200      2.200 peak 23502 weight 0.10000E+01 volume 0.14819E+01 ppm1 1.812 ppm2 0.171
ASSI {23522}
(( segid "PROT" and resid 28 and name HB1 ))
(( segid "PROT" and resid 32 and name HE3 ))
3.500      3.100      2.000 peak 23522 weight 0.10000E+01 volume 0.55110E+00 ppm1 3.026 ppm2 7.342
ASSI {23582}
(( segid "PROT" and resid 19 and name HB2 ))
(( segid "PROT" and resid 19 and name HE1 ))
3.300      2.700      2.200 peak 23582 weight 0.10000E+01 volume 0.79520E+00 ppm1 1.404 ppm2 2.976
ASSI {23592}
(( segid "PROT" and resid 19 and name HB1 ))
(( segid "PROT" and resid 19 and name HE1 ))
3.200      2.600      2.300 peak 23592 weight 0.10000E+01 volume 0.88430E+00 ppm1 1.738 ppm2 2.961
ASSI {23652}
(( segid "PROT" and resid 38 and name HB ))
(( segid "PROT" and resid 50 and name HG2% ))
3.400      2.900      2.100 peak 23652 weight 0.10000E+01 volume 0.65450E+00 ppm1 1.073 ppm2 0.414
ASSI {23752}
(( segid "PROT" and resid 75 and name HB2 ))
(( segid "PROT" and resid 115 and name HD1% ))
3.500      3.100      2.000 peak 23752 weight 0.10000E+01 volume 0.54290E+00 ppm1 2.655 ppm2 0.763
OR {23752}
(( segid "PROT" and resid 75 and name HB2 ))
(( segid "PROT" and resid 115 and name HD2% ))
ASSI {23762}
(( segid "PROT" and resid 59 and name HG1 ))
(( segid "PROT" and resid 62 and name HG1 ))
3.500      3.100      2.000 peak 23762 weight 0.10000E+01 volume 0.57320E+00 ppm1 2.654 ppm2 1.727
ASSI {23852}
(( segid "PROT" and resid 49 and name HB ))
(( segid "PROT" and resid 46 and name HA ))
3.400      2.900      2.100 peak 23852 weight 0.10000E+01 volume 0.63410E+00 ppm1 1.926 ppm2 3.509
ASSI {23872}
(( segid "PROT" and resid 49 and name HB ))
(( segid "PROT" and resid 84 and name HB1 ))
3.400      2.900      2.100 peak 23872 weight 0.10000E+01 volume 0.68110E+00 ppm1 1.930 ppm2 3.009
ASSI {23912}
(( segid "PROT" and resid 49 and name HB ))
(( segid "PROT" and resid 88 and name HD% ))
3.300      2.700      2.200 peak 23912 weight 0.10000E+01 volume 0.79550E+00 ppm1 1.932 ppm2 6.968
ASSI {24042}
(( segid "PROT" and resid 110 and name HB ))
(( segid "PROT" and resid 113 and name HB% ))
3.200      2.600      2.300 peak 24042 weight 0.10000E+01 volume 0.99190E+00 ppm1 1.794 ppm2 1.406
ASSI {24092}
(( segid "PROT" and resid 21 and name HB ))
(( segid "PROT" and resid 17 and name HG2% ))
3.400      2.900      2.100 peak 24092 weight 0.10000E+01 volume 0.66400E+00 ppm1 1.950 ppm2 1.168
ASSI {24192}
(( segid "PROT" and resid 101 and name HB ))
(( segid "PROT" and resid 102 and name HD1% ))
3.500      3.100      2.000 peak 24192 weight 0.10000E+01 volume 0.56440E+00 ppm1 1.947 ppm2 0.778
OR {24192}
(( segid "PROT" and resid 101 and name HB ))
(( segid "PROT" and resid 102 and name HD2% ))
ASSI {24262}
(( segid "PROT" and resid 18 and name HB2 ))
(( segid "PROT" and resid 74 and name HE% ))
3.400      2.900      2.100 peak 24262 weight 0.10000E+01 volume 0.67690E+00 ppm1 0.347 ppm2 6.978
ASSI {24492}
(( segid "PROT" and resid 51 and name HD1 ))
(( segid "PROT" and resid 80 and name HD1 ))
2.400      1.400      1.400 peak 24492 weight 0.10000E+01 volume 0.59941E+01 ppm1 3.020 ppm2 3.406
ASSI {24622}
(( segid "PROT" and resid 43 and name HA ))
(( segid "PROT" and resid 42 and name HA ))
3.400      2.900      2.100 peak 24622 weight 0.10000E+01 volume 0.67930E+00 ppm1 4.987 ppm2 4.480
ASSI {24632}
(( segid "PROT" and resid 33 and name HD1 ))
(( segid "PROT" and resid 32 and name HE3 ))
3.300      2.700      2.200 peak 24632 weight 0.10000E+01 volume 0.73690E+00 ppm1 2.265 ppm2 7.320
ASSI {24672}
(( segid "PROT" and resid 8 and name HD2 ))
(( segid "PROT" and resid 115 and name HD1% ))
3.300      2.700      2.200 peak 24672 weight 0.10000E+01 volume 0.74890E+00 ppm1 3.713 ppm2 0.781
OR {24672}
(( segid "PROT" and resid 8 and name HD2 ))
(( segid "PROT" and resid 115 and name HD2% ))
ASSI {24682}
(( segid "PROT" and resid 89 and name HA ))
(( segid "PROT" and resid 90 and name HB2 ))
3.100      2.400      2.400 peak 24682 weight 0.10000E+01 volume 0.11403E+01 ppm1 5.093 ppm2 2.202
ASSI {24902}
(( segid "PROT" and resid 34 and name HA ))
(( segid "PROT" and resid 102 and name HD1% ))

```

```

3.400      2.900      2.100 peak 24902 weight 0.10000E+01 volume 0.62620E+00 ppm1 5.008 ppm2 0.773
ASSI {24942}
(( segid "PROT" and resid 100 and name HA ))
(( segid "PROT" and resid 86 and name HE2 ))
3.100      2.400      2.400 peak 24942 weight 0.10000E+01 volume 0.12073E+01 ppm1 4.380 ppm2 2.466
OR {24942}
(( segid "PROT" and resid 100 and name HA ))
(( segid "PROT" and resid 86 and name HE1 ))
ASSI {24972}
(( segid "PROT" and resid 39 and name HA ))
(( segid "PROT" and resid 39 and name HB2 ))
2.500      1.600      1.600 peak 24972 weight 0.10000E+01 volume 0.46002E+01 ppm1 4.444 ppm2 1.935
ASSI {25082}
(( segid "PROT" and resid 77 and name HA ))
(( segid "PROT" and resid 59 and name HE% ))
3.300      2.700      2.200 peak 25082 weight 0.10000E+01 volume 0.74310E+00 ppm1 4.400 ppm2 1.310
ASSI {25282}
(( segid "PROT" and resid 26 and name HA ))
(( segid "PROT" and resid 25 and name HG2% ))
2.900      2.100      2.100 peak 25282 weight 0.10000E+01 volume 0.18601E+01 ppm1 3.928 ppm2 1.068
ASSI {25372}
(( segid "PROT" and resid 16 and name HB2 ))
(( segid "PROT" and resid 19 and name HD1 ))
3.100      2.400      2.400 peak 25372 weight 0.10000E+01 volume 0.10814E+01 ppm1 3.953 ppm2 1.636
ASSI {25382}
(( segid "PROT" and resid 46 and name HA ))
(( segid "PROT" and resid 38 and name HG2% ))
3.600      3.200      1.900 peak 25382 weight 0.10000E+01 volume 0.49500E+00 ppm1 3.505 ppm2 -0.005
ASSI {25562}
(( segid "PROT" and resid 38 and name HA ))
(( segid "PROT" and resid 39 and name HB2 ))
3.400      2.900      2.100 peak 25562 weight 0.10000E+01 volume 0.71250E+00 ppm1 3.491 ppm2 1.940
ASSI {25622}
(( segid "PROT" and resid 21 and name HA ))
(( segid "PROT" and resid 17 and name HG2% ))
3.400      2.900      2.100 peak 25622 weight 0.10000E+01 volume 0.65110E+00 ppm1 3.795 ppm2 1.169
ASSI {25702}
(( segid "PROT" and resid 25 and name HA ))
(( segid "PROT" and resid 26 and name HB1 ))
3.500      3.100      2.000 peak 25702 weight 0.10000E+01 volume 0.52050E+00 ppm1 3.863 ppm2 1.890
ASSI {25732}
(( segid "PROT" and resid 17 and name HB ))
(( segid "PROT" and resid 115 and name HD2% ))
3.200      2.600      2.300 peak 25732 weight 0.10000E+01 volume 0.89690E+00 ppm1 4.292 ppm2 0.754
OR {25732}
(( segid "PROT" and resid 17 and name HB ))
(( segid "PROT" and resid 115 and name HD1% ))
ASSI {25822}
(( segid "PROT" and resid 43 and name HA ))
(( segid "PEPT" and resid 204 and name HA ))
3.400      2.900      2.100 peak 25822 weight 0.10000E+01 volume 0.68700E+00 ppm1 4.984 ppm2 4.392
ASSI {26032}
(( segid "PROT" and resid 99 and name HB% ))
(( segid "PROT" and resid 96 and name HE% ))
3.200      2.600      2.300 peak 26032 weight 0.10000E+01 volume 0.87540E+00 ppm1 1.670 ppm2 7.060
ASSI {26052}
(( segid "PROT" and resid 113 and name HA ))
(( segid "PROT" and resid 21 and name HD1% ))
3.500      3.100      2.000 peak 26052 weight 0.10000E+01 volume 0.52350E+00 ppm1 4.340 ppm2 0.652
ASSI {26212}
(( segid "PROT" and resid 18 and name HD1% ))
(( segid "PROT" and resid 78 and name HD1% ))
3.600      3.200      1.900 peak 26212 weight 0.10000E+01 volume 0.49240E+00 ppm1 0.517 ppm2 0.083
ASSI {26252}
(( segid "PROT" and resid 94 and name HA ))
(( segid "PROT" and resid 93 and name HA ))
3.100      2.400      2.400 peak 26252 weight 0.10000E+01 volume 0.11336E+01 ppm1 4.226 ppm2 4.535
ASSI {26402}
(( segid "PROT" and resid 33 and name HD2 ))
(( segid "PROT" and resid 34 and name HD% ))
3.100      2.400      2.400 peak 26402 weight 0.10000E+01 volume 0.10972E+01 ppm1 1.563 ppm2 7.197
OR {26402}
(( segid "PROT" and resid 33 and name HD2 ))
(( segid "PROT" and resid 34 and name HE% ))
ASSI {26472}
(( segid "PROT" and resid 35 and name HE% ))
(( segid "PROT" and resid 34 and name HB2 ))
3.400      2.900      2.100 peak 26472 weight 0.10000E+01 volume 0.63450E+00 ppm1 2.211 ppm2 2.595
ASSI {26652}
(( segid "PROT" and resid 18 and name HA ))
(( segid "PROT" and resid 22 and name HB1 ))
3.500      3.100      2.000 peak 26652 weight 0.10000E+01 volume 0.57230E+00 ppm1 3.303 ppm2 2.087
ASSI {26672}
(( segid "PROT" and resid 6 and name HA ))
(( segid "PROT" and resid 117 and name HB1 ))
3.400      2.900      2.100 peak 26672 weight 0.10000E+01 volume 0.65680E+00 ppm1 4.374 ppm2 2.708
ASSI {26742}
(( segid "PROT" and resid 80 and name HB2 ))
(( segid "PROT" and resid 81 and name HA ))

```



```

ASSI { 353}
  (( segid "PEPT" and resid 207 and name HN ))
  (( segid "PEPT" and resid 206 and name HG1 ))
  3.300 2.700 2.200 peak 353 weight 0.10000E+01 volume 0.29440E+01 ppm1 8.451 ppm2 1.440
ASSI { 363}
  (( segid "PEPT" and resid 205 and name HZ ))
  (( segid "PEPT" and resid 205 and name HH% ))
  2.100 1.100 1.100 peak 363 weight 0.10000E+01 volume 0.50754E+02 ppm1 7.876 ppm2 1.872
ASSI { 373}
  (( segid "PEPT" and resid 205 and name HZ ))
  (( segid "PEPT" and resid 204 and name HN ))
  3.200 2.600 2.300 peak 373 weight 0.10000E+01 volume 0.40017E+01 ppm1 7.881 ppm2 8.105
ASSI { 144}
  (( segid "PEPT" and resid 202 and name HD% ))
  (( segid "PEPT" and resid 202 and name HB2 ))
  2.700 1.800 1.800 peak 144 weight 0.10000E+01 volume 0.25326E+01 ppm1 7.133 ppm2 2.913
ASSI { 154}
  (( segid "PEPT" and resid 202 and name HD% ))
  (( segid "PEPT" and resid 202 and name HB1 ))
  2.700 1.800 1.800 peak 154 weight 0.10000E+01 volume 0.25762E+01 ppm1 7.134 ppm2 3.130
ASSI { 164}
  (( segid "PEPT" and resid 202 and name HD% ))
  (( segid "PEPT" and resid 202 and name HA ))
  2.700 1.800 1.800 peak 164 weight 0.10000E+01 volume 0.25087E+01 ppm1 7.134 ppm2 4.622
ASSI { 184}
  (( segid "PEPT" and resid 205 and name HZ ))
  (( segid "PEPT" and resid 205 and name HG1 ))
  2.900 2.100 2.100 peak 184 weight 0.10000E+01 volume 0.14841E+01 ppm1 7.882 ppm2 1.321
ASSI { 194}
  (( segid "PROT" and resid 88 and name HD% ))
  (( segid "PEPT" and resid 202 and name HB2 ))
  3.800 3.600 1.700 peak 194 weight 0.10000E+01 volume 0.29670E+00 ppm1 7.008 ppm2 2.919
ASSI { 214}
  (( segid "PROT" and resid 89 and name HD22 ))
  (( segid "PEPT" and resid 205 and name HB1 ))
  3.400 2.900 2.100 peak 214 weight 0.10000E+01 volume 0.58630E+00 ppm1 7.822 ppm2 3.090
ASSI { 264}
  (( segid "PEPT" and resid 209 and name HN ))
  (( segid "PEPT" and resid 209 and name HB2 ))
  3.500 3.100 2.000 peak 264 weight 0.10000E+01 volume 0.47310E+00 ppm1 8.499 ppm2 1.974
ASSI { 5}
  (( segid "PEPT" and resid 202 and name HD% ))
  (( segid "PROT" and resid 49 and name HG1% ))
  2.900 2.100 2.100 peak 5 weight 0.11000E+02 volume 0.17073E+01 ppm1 7.134 ppm2 0.978
ASSI { 95}
  (( segid "PEPT" and resid 202 and name HB2 ))
  (( segid "PROT" and resid 49 and name HG1% ))
  3.300 2.700 2.200 peak 95 weight 0.11000E+02 volume 0.87280E+00 ppm1 2.894 ppm2 0.977
ASSI { 125}
  (( segid "PEPT" and resid 206 and name HG1 ))
  (( segid "PROT" and resid 43 and name HB% ))
  3.200 2.600 2.300 peak 125 weight 0.10000E+01 volume 0.10680E+01 ppm1 1.462 ppm2 1.047
ASSI { 135}
  (( segid "PEPT" and resid 204 and name HB2 ))
  (( segid "PROT" and resid 43 and name HB% ))
  3.100 2.400 2.400 peak 135 weight 0.10000E+01 volume 0.11770E+01 ppm1 1.778 ppm2 1.036
ASSI { 145}
  (( segid "PEPT" and resid 205 and name HB1 ))
  (( segid "PROT" and resid 38 and name HG1% ))
  3.300 2.700 2.200 peak 145 weight 0.10000E+01 volume 0.89880E+00 ppm1 3.068 ppm2 0.458
ASSI { 155}
  (( segid "PEPT" and resid 205 and name HH% ))
  (( segid "PROT" and resid 38 and name HG1% ))
  2.200 1.200 1.200 peak 155 weight 0.10000E+01 volume 0.87158E+01 ppm1 1.893 ppm2 0.463
ASSI { 165}
  (( segid "PEPT" and resid 205 and name HH% ))
  (( segid "PROT" and resid 38 and name HA ))
  3.200 2.600 2.300 peak 165 weight 0.10000E+01 volume 0.10856E+01 ppm1 1.890 ppm2 3.506
ASSI { 195}
  (( segid "PEPT" and resid 208 and name HB1 ))
  (( segid "PROT" and resid 42 and name HG1 ))
  3.200 2.600 2.300 peak 195 weight 0.10000E+01 volume 0.96050E+00 ppm1 1.781 ppm2 2.325
ASSI { 205}
  (( segid "PEPT" and resid 209 and name HB1 ))
  (( segid "PROT" and resid 42 and name HG1 ))
  3.100 2.400 2.400 peak 205 weight 0.10000E+01 volume 0.11438E+01 ppm1 2.109 ppm2 2.322
ASSI { 215}
  (( segid "PEPT" and resid 209 and name HG1 ))
  (( segid "PROT" and resid 42 and name HG2 ))
  3.500 3.100 2.000 peak 215 weight 0.10000E+01 volume 0.54870E+00 ppm1 2.343 ppm2 2.245
ASSI { 255}
  (( segid "PEPT" and resid 208 and name HA ))
  (( segid "PROT" and resid 42 and name HG1 ))
  2.900 2.100 2.100 peak 255 weight 0.10000E+01 volume 0.16895E+01 ppm1 4.326 ppm2 2.322
ASSI { 275}
  (( segid "PEPT" and resid 209 and name HE22 ))
  (( segid "PROT" and resid 42 and name HG2 ))
  3.500 3.100 2.000 peak 275 weight 0.10000E+01 volume 0.56640E+00 ppm1 6.869 ppm2 2.323
ASSI { 375}

```

```

(( segid "PEPT" and resid 208 and name HA ))
(( segid "PROT" and resid 42 and name HB1 ))
3.100 2.400 2.400 peak 375 weight 0.10000E+01 volume 0.12561E+01 ppm1 4.319 ppm2 2.168
ASSI { 405}
(( segid "PEPT" and resid 208 and name HA ))
(( segid "PROT" and resid 42 and name HB2 ))
3.200 2.600 2.300 peak 405 weight 0.10000E+01 volume 0.10728E+01 ppm1 4.319 ppm2 2.075
ASSI { 425}
(( segid "PEPT" and resid 209 and name HE22))
(( segid "PROT" and resid 42 and name HB2 ))
3.200 2.600 2.300 peak 425 weight 0.10000E+01 volume 0.10307E+01 ppm1 6.870 ppm2 2.072
ASSI { 445}
(( segid "PEPT" and resid 205 and name HH% ))
(( segid "PROT" and resid 33 and name HB2 ))
3.300 2.700 2.200 peak 445 weight 0.10000E+01 volume 0.84810E+00 ppm1 1.886 ppm2 -0.445
ASSI { 525}
(( segid "PEPT" and resid 205 and name HH% ))
(( segid "PROT" and resid 81 and name HG1% ))
2.300 2.300 2.200 peak 525 weight 0.10000E+01 volume 0.81157E+01 ppm1 1.885 ppm2 0.496
ASSI { 535}
(( segid "PEPT" and resid 203 and name HN ))
(( segid "PROT" and resid 50 and name HD1% ))
3.600 3.200 1.900 peak 535 weight 0.10000E+01 volume 0.45510E+00 ppm1 8.245 ppm2 0.597
ASSI { 245}
(( segid "PROT" and resid 42 and name HG2 ))
(( segid "PROT" and resid 41 and name HA ))
3.200 2.600 2.300 peak 245 weight 0.10000E+01 volume 0.95560E+00 ppm1 2.323 ppm2 4.076
OR { 245}
(( segid "PROT" and resid 42 and name HG1 ))
(( segid "PROT" and resid 41 and name HA ))
ASSI { 265}
(( segid "PROT" and resid 42 and name HG2 ))
(( segid "PROT" and resid 42 and name HA ))
3.300 2.700 2.200 peak 265 weight 0.10000E+01 volume 0.85890E+00 ppm1 2.339 ppm2 4.484
OR { 265}
(( segid "PROT" and resid 42 and name HG1 ))
(( segid "PROT" and resid 42 and name HA ))
ASSI { 465}
(( segid "PROT" and resid 33 and name HB2 ))
(( segid "PROT" and resid 95 and name HA ))
3.500 3.100 2.000 peak 465 weight 0.10000E+01 volume 0.59690E+00 ppm1 -0.448 ppm2 3.636
ASSI { 6}
(( segid "PEPT" and resid 205 and name HB1 ))
(( segid "PROT" and resid 95 and name HE% ))
2.900 2.100 2.100 peak 6 weight 0.11000E+02 volume 0.20642E+01 ppm1 1.768 ppm2 7.010
ASSI { 16}
(( segid "PEPT" and resid 205 and name HB1 ))
(( segid "PROT" and resid 88 and name HE% ))
3.200 2.600 2.300 peak 16 weight 0.11000E+02 volume 0.12360E+01 ppm1 1.782 ppm2 6.634
ASSI { 26}
(( segid "PEPT" and resid 205 and name HD1 ))
(( segid "PROT" and resid 88 and name HE% ))
3.000 2.200 2.200 peak 26 weight 0.11000E+02 volume 0.18014E+01 ppm1 1.431 ppm2 6.631
ASSI { 36}
(( segid "PEPT" and resid 205 and name HG1 ))
(( segid "PROT" and resid 88 and name HE% ))
3.100 2.400 2.400 peak 36 weight 0.11000E+02 volume 0.15181E+01 ppm1 1.327 ppm2 6.632
ASSI { 46}
(( segid "PEPT" and resid 202 and name HB1 ))
(( segid "PROT" and resid 88 and name HE% ))
3.200 2.600 2.300 peak 46 weight 0.11000E+02 volume 0.11426E+01 ppm1 3.114 ppm2 6.636
ASSI { 56}
(( segid "PEPT" and resid 205 and name HD1 ))
(( segid "PROT" and resid 95 and name HE% ))
3.500 3.100 2.000 peak 56 weight 0.11000E+02 volume 0.77060E+00 ppm1 1.430 ppm2 7.010
ASSI { 66}
(( segid "PEPT" and resid 205 and name HG1 ))
(( segid "PROT" and resid 95 and name HE% ))
3.600 3.200 1.900 peak 66 weight 0.11000E+02 volume 0.58800E+00 ppm1 1.320 ppm2 7.010
ASSI { 76}
(( segid "PEPT" and resid 205 and name HG2 ))
(( segid "PROT" and resid 95 and name HE% ))
3.700 3.400 1.800 peak 76 weight 0.11000E+02 volume 0.50830E+00 ppm1 1.160 ppm2 7.015
ASSI { 86}
(( segid "PEPT" and resid 205 and name HH% ))
(( segid "PROT" and resid 95 and name HE% ))
3.200 2.600 2.300 peak 86 weight 0.11000E+02 volume 0.11871E+01 ppm1 1.914 ppm2 7.010
ASSI { 96}
(( segid "PEPT" and resid 205 and name HE1 ))
(( segid "PROT" and resid 95 and name HE% ))
3.500 3.100 2.000 peak 96 weight 0.11000E+02 volume 0.68560E+00 ppm1 3.113 ppm2 7.019
ASSI { 106}
(( segid "PEPT" and resid 205 and name HA ))
(( segid "PROT" and resid 95 and name HE% ))
3.400 2.900 2.100 peak 106 weight 0.11000E+02 volume 0.80400E+00 ppm1 4.325 ppm2 7.010
ASSI { 116}
(( segid "PEPT" and resid 202 and name HB1 ))
(( segid "PROT" and resid 88 and name HD% ))
3.200 2.600 2.300 peak 116 weight 0.11000E+02 volume 0.12205E+01 ppm1 3.122 ppm2 6.962

```

```

ASSI { 136}
(( segid "PEPT" and resid 205 and name HD1 ))
( segid "PROT" and resid 88 and name HD% )
3.600 3.200 1.900 peak 136 weight 0.11000E+02 volume 0.60120E+00 ppm1 1.436 ppm2 6.961
ASSI { 146}
(( segid "PEPT" and resid 205 and name HG1 ))
( segid "PROT" and resid 88 and name HD% )
3.600 3.200 1.900 peak 146 weight 0.11000E+02 volume 0.61310E+00 ppm1 1.326 ppm2 6.959
ASSI { 156}
( segid "PEPT" and resid 205 and name HH% )
( segid "PROT" and resid 95 and name HD% )
2.900 2.100 2.100 peak 156 weight 0.11000E+02 volume 0.20765E+01 ppm1 1.930 ppm2 6.845
ASSI { 126}
( segid "PROT" and resid 88 and name HD% )
(( segid "PROT" and resid 88 and name HB1 ))
3.600 3.200 1.900 peak 126 weight 0.10000E+01 volume 0.59050E+00 ppm1 6.959 ppm2 2.946
OR { 126}
( segid "PROT" and resid 88 and name HD% )
(( segid "PROT" and resid 88 and name HB2 ))

```

Table 14 Ambiguous NOE Distance Restraints

```

ASSI { 1101}
(( segid "PROT" and resid 102 and name HN ))
( segid "PROT" and resid 31 and name HB% )
3.500 3.100 2.000 peak 1101 weight 0.10000E+01 volume 0.13797E+01 ppm1 8.519 ppm2 1.706
OR { 1101}
(( segid "PROT" and resid 102 and name HN ))
(( segid "PROT" and resid 104 and name HD1 ))
ASSI { 1211}
(( segid "PROT" and resid 103 and name HN ))
(( segid "PROT" and resid 104 and name HA ))
3.200 2.600 2.300 peak 1211 weight 0.10000E+01 volume 0.23779E+01 ppm1 8.042 ppm2 4.062
OR { 1211}
(( segid "PROT" and resid 46 and name HN ))
(( segid "PROT" and resid 48 and name HA ))
ASSI { 1311}
(( segid "PROT" and resid 103 and name HN ))
(( segid "PROT" and resid 98 and name HA ))
3.200 2.600 2.300 peak 1311 weight 0.10000E+01 volume 0.24662E+01 ppm1 8.037 ppm2 4.220
OR { 1311}
(( segid "PROT" and resid 103 and name HN ))
(( segid "PROT" and resid 82 and name HA ))
ASSI { 2161}
(( segid "PROT" and resid 112 and name HN ))
( segid "PROT" and resid 115 and name HD2% )
3.400 2.900 2.100 peak 2161 weight 0.10000E+01 volume 0.15055E+01 ppm1 8.057 ppm2 0.824
OR { 2161}
(( segid "PROT" and resid 112 and name HN ))
(( segid "PROT" and resid 109 and name HG1 ))
OR { 2161}
(( segid "PROT" and resid 112 and name HN ))
( segid "PROT" and resid 116 and name HG2% )
OR { 2161}
(( segid "PROT" and resid 112 and name HN ))
( segid "PROT" and resid 116 and name HD1% )
ASSI { 2501}
(( segid "PROT" and resid 106 and name HN ))
(( segid "PROT" and resid 102 and name HG ))
3.600 3.200 1.900 peak 2501 weight 0.10000E+01 volume 0.11395E+01 ppm1 9.149 ppm2 1.562
OR { 2501}
(( segid "PROT" and resid 106 and name HN ))
(( segid "PROT" and resid 109 and name HB2 ))
OR { 2501}
(( segid "PROT" and resid 106 and name HN ))
(( segid "PROT" and resid 104 and name HG1 ))
ASSI { 2711}
(( segid "PROT" and resid 17 and name HN ))
( segid "PROT" and resid 18 and name HD1% )
3.300 2.700 2.200 peak 2711 weight 0.10000E+01 volume 0.19671E+01 ppm1 8.065 ppm2 0.730
OR { 2711}
(( segid "PROT" and resid 17 and name HN ))
( segid "PROT" and resid 115 and name HD1% )
ASSI { 2731}
(( segid "PROT" and resid 40 and name HN ))
(( segid "PROT" and resid 39 and name HB1 ))
2.700 1.800 1.800 peak 2731 weight 0.10000E+01 volume 0.59635E+01 ppm1 8.059 ppm2 3.194
OR { 2731}
(( segid "PROT" and resid 17 and name HN ))
(( segid "PROT" and resid 15 and name HB1 ))
ASSI { 2771}
(( segid "PROT" and resid 17 and name HN ))
(( segid "PROT" and resid 18 and name HB1 ))
3.200 2.600 2.300 peak 2771 weight 0.10000E+01 volume 0.21928E+01 ppm1 8.060 ppm2 1.555
OR { 2771}
(( segid "PROT" and resid 17 and name HN ))
(( segid "PROT" and resid 14 and name HB2 ))
ASSI { 4121}
(( segid "PROT" and resid 78 and name HN ))
(( segid "PROT" and resid 79 and name HB2 ))
3.200 2.600 2.300 peak 4121 weight 0.10000E+01 volume 0.21825E+01 ppm1 7.368 ppm2 2.089
OR { 4121}
(( segid "PROT" and resid 78 and name HN ))
( segid "PROT" and resid 75 and name HE% )
OR { 4121}
(( segid "PROT" and resid 96 and name HN ))
(( segid "PROT" and resid 97 and name HB1 ))
OR { 4121}
(( segid "PROT" and resid 77 and name HN ))
(( segid "PROT" and resid 79 and name HB2 ))
OR { 4121}
(( segid "PROT" and resid 78 and name HN ))
(( segid "PROT" and resid 54 and name HB1 ))
OR { 4121}
(( segid "PROT" and resid 77 and name HN ))
(( segid "PROT" and resid 54 and name HB1 ))
ASSI { 4331}

```

```

(( segid "PROT" and resid 78 and name HN ))
(( segid "PROT" and resid 81 and name HB ))
3.300 2.700 2.200 peak 4331 weight 0.10000E+01 volume 0.21033E+01 ppm1 7.382 ppm2 1.417
OR { 4331}
(( segid "PROT" and resid 77 and name HN ))
(( segid "PROT" and resid 81 and name HB ))
ASSI { 4731}
(( segid "PROT" and resid 15 and name HN ))
(( segid "PROT" and resid 16 and name HB2 ))
3.300 2.700 2.200 peak 4731 weight 0.10000E+01 volume 0.19906E+01 ppm1 7.992 ppm2 3.907
OR { 4731}
(( segid "PROT" and resid 15 and name HN ))
(( segid "PROT" and resid 17 and name HA ))
OR { 4731}
(( segid "PROT" and resid 15 and name HN ))
(( segid "PROT" and resid 11 and name HD1 ))
ASSI { 6431}
(( segid "PROT" and resid 113 and name HN ))
(( segid "PROT" and resid 111 and name HG2 ))
3.200 2.600 2.300 peak 6431 weight 0.10000E+01 volume 0.23779E+01 ppm1 7.627 ppm2 1.290
OR { 6431}
(( segid "PROT" and resid 113 and name HN ))
(( segid "PROT" and resid 116 and name HG11))
ASSI { 6531}
(( segid "PROT" and resid 104 and name HN ))
(( segid "PROT" and resid 102 and name HB1 ))
3.500 3.100 2.000 peak 6531 weight 0.10000E+01 volume 0.12949E+01 ppm1 7.168 ppm2 1.396
OR { 6531}
(( segid "PROT" and resid 35 and name HN ))
(( segid "PROT" and resid 56 and name HB2 ))
ASSI { 6731}
(( segid "PROT" and resid 35 and name HN ))
(( segid "PROT" and resid 56 and name HD18))
3.400 2.900 2.100 peak 6731 weight 0.10000E+01 volume 0.15507E+01 ppm1 7.148 ppm2 0.971
OR { 6731}
(( segid "PROT" and resid 104 and name HN ))
(( segid "PROT" and resid 101 and name HG2%))
ASSI { 7671}
(( segid "PROT" and resid 82 and name HN ))
(( segid "PROT" and resid 83 and name HG2%))
3.200 2.600 2.300 peak 7671 weight 0.10000E+01 volume 0.24316E+01 ppm1 6.396 ppm2 1.323
OR { 7671}
(( segid "PROT" and resid 82 and name HN ))
(( segid "PROT" and resid 54 and name HB2 ))
OR { 7671}
(( segid "PROT" and resid 82 and name HN ))
(( segid "PROT" and resid 103 and name HB2 ))
ASSI { 7851}
(( segid "PROT" and resid 98 and name HN ))
(( segid "PROT" and resid 30 and name HB1 ))
3.400 2.900 2.100 peak 7851 weight 0.10000E+01 volume 0.15319E+01 ppm1 8.470 ppm2 4.315
OR { 7851}
(( segid "PROT" and resid 98 and name HN ))
(( segid "PROT" and resid 100 and name HA ))
ASSI { 8591}
(( segid "PROT" and resid 95 and name HN ))
(( segid "PROT" and resid 97 and name HG1 ))
3.300 2.700 2.200 peak 8591 weight 0.10000E+01 volume 0.18918E+01 ppm1 7.964 ppm2 1.794
OR { 8591}
(( segid "PROT" and resid 65 and name HN ))
(( segid "PROT" and resid 64 and name HD1 ))
OR { 8591}
(( segid "PROT" and resid 60 and name HN ))
(( segid "PROT" and resid 22 and name HG ))
ASSI { 8701}
(( segid "PROT" and resid 56 and name HN ))
(( segid "PROT" and resid 25 and name HG2%))
3.400 2.900 2.100 peak 8701 weight 0.10000E+01 volume 0.15401E+01 ppm1 9.133 ppm2 1.035
OR { 8701}
(( segid "PROT" and resid 56 and name HN ))
(( segid "PROT" and resid 22 and name HD2%))
ASSI {11861}
(( segid "PROT" and resid 24 and name HE22))
(( segid "PROT" and resid 24 and name HG2 ))
3.700 3.400 1.800 peak 11861 weight 0.10000E+01 volume 0.91710E+00 ppm1 6.901 ppm2 2.481
OR {11861}
(( segid "PROT" and resid 24 and name HE22))
(( segid "PROT" and resid 109 and name HE2 ))
ASSI {12111}
(( segid "PROT" and resid 68 and name HN ))
(( segid "PROT" and resid 66 and name HG1 ))
3.800 3.600 1.700 peak 12111 weight 0.10000E+01 volume 0.85210E+00 ppm1 8.011 ppm2 1.643
OR {12111}
(( segid "PROT" and resid 68 and name HN ))
(( segid "PROT" and resid 18 and name HG ))
ASSI {12191}
(( segid "PROT" and resid 89 and name HN ))
(( segid "PEPT" and resid 203 and name HA1 ))
3.700 3.400 1.800 peak 12191 weight 0.10000E+01 volume 0.10424E+01 ppm1 8.114 ppm2 3.902

```

```

OR {12191}
  (( segid "PROT" and resid 89 and name HN ))
  (( segid "PROT" and resid 83 and name HA ))
OR {12191}
  (( segid "PROT" and resid 89 and name HN ))
  (( segid "PROT" and resid 50 and name HA ))
ASSI {12361}
  (( segid "PROT" and resid 69 and name HN ))
  (( segid "PROT" and resid 70 and name HB1 ))
  3.700 3.400 1.800 peak 12361 weight 0.10000E+01 volume 0.10231E+01 ppm1 7.707 ppm2 4.230
OR {12361}
  (( segid "PROT" and resid 69 and name HN ))
  (( segid "PROT" and resid 73 and name HA ))
ASSI {12371}
  (( segid "PROT" and resid 69 and name HN ))
  (( segid "PROT" and resid 63 and name HD2% ))
  3.500 3.100 2.000 peak 12371 weight 0.10000E+01 volume 0.14140E+01 ppm1 7.709 ppm2 1.055
OR {12371}
  (( segid "PROT" and resid 69 and name HN ))
  (( segid "PROT" and resid 62 and name HB2 ))
ASSI {12571}
  (( segid "PROT" and resid 110 and name HN ))
  (( segid "PROT" and resid 75 and name HE% ))
  3.600 3.200 1.900 peak 12571 weight 0.10000E+01 volume 0.12095E+01 ppm1 8.119 ppm2 2.066
OR {12571}
  (( segid "PROT" and resid 110 and name HN ))
  (( segid "PROT" and resid 112 and name HB1 ))
ASSI {12731}
  (( segid "PROT" and resid 107 and name HN ))
  (( segid "PROT" and resid 111 and name HB2 ))
  3.700 3.400 1.800 peak 12731 weight 0.10000E+01 volume 0.10305E+01 ppm1 8.400 ppm2 1.726
OR {12731}
  (( segid "PROT" and resid 107 and name HN ))
  (( segid "PROT" and resid 104 and name HD1 ))
OR {12731}
  (( segid "PROT" and resid 107 and name HN ))
  (( segid "PROT" and resid 109 and name HB1 ))
ASSI {12741}
  (( segid "PROT" and resid 107 and name HN ))
  (( segid "PROT" and resid 109 and name HG1 ))
  3.700 3.400 1.800 peak 12741 weight 0.10000E+01 volume 0.94540E+00 ppm1 8.398 ppm2 0.803
OR {12741}
  (( segid "PROT" and resid 107 and name HN ))
  (( segid "PROT" and resid 116 and name HD1% ))
ASSI {12761}
  (( segid "PROT" and resid 19 and name HN ))
  (( segid "PROT" and resid 19 and name HE1 ))
  3.700 3.400 1.800 peak 12761 weight 0.10000E+01 volume 0.95080E+00 ppm1 8.574 ppm2 2.934
OR {12761}
  (( segid "PROT" and resid 19 and name HN ))
  (( segid "PROT" and resid 68 and name HB2 ))
ASSI {12961}
  (( segid "PROT" and resid 78 and name HN ))
  (( segid "PROT" and resid 74 and name HD% ))
  3.800 3.600 1.700 peak 12961 weight 0.10000E+01 volume 0.85250E+00 ppm1 7.386 ppm2 6.387
OR {12961}
  (( segid "PROT" and resid 77 and name HN ))
  (( segid "PROT" and resid 74 and name HD% ))
ASSI {13011}
  (( segid "PROT" and resid 25 and name HN ))
  (( segid "PROT" and resid 31 and name HB% ))
  3.600 3.200 1.900 peak 13011 weight 0.10000E+01 volume 0.11117E+01 ppm1 8.563 ppm2 1.722
OR {13011}
  (( segid "PROT" and resid 25 and name HN ))
  (( segid "PROT" and resid 22 and name HB2 ))
ASSI {13031}
  (( segid "PROT" and resid 101 and name HN ))
  (( segid "PROT" and resid 104 and name HN ))
  3.700 3.400 1.800 peak 13031 weight 0.10000E+01 volume 0.10135E+01 ppm1 8.016 ppm2 7.190
OR {13031}
  (( segid "PROT" and resid 101 and name HN ))
  (( segid "PROT" and resid 34 and name HE% ))
ASSI {13101}
  (( segid "PROT" and resid 22 and name HN ))
  (( segid "PROT" and resid 23 and name HB1 ))
  3.800 3.600 1.700 peak 13101 weight 0.10000E+01 volume 0.88170E+00 ppm1 8.853 ppm2 2.327
OR {13101}
  (( segid "PROT" and resid 22 and name HN ))
  (( segid "PROT" and resid 63 and name HB1 ))
ASSI {13211}
  (( segid "PROT" and resid 62 and name HN ))
  (( segid "PROT" and resid 67 and name HB1 ))
  3.600 3.200 1.900 peak 13211 weight 0.10000E+01 volume 0.10881E+01 ppm1 8.378 ppm2 2.990
OR {13211}
  (( segid "PROT" and resid 62 and name HN ))
  (( segid "PROT" and resid 65 and name HB1 ))
OR {13211}
  (( segid "PROT" and resid 62 and name HN ))
  (( segid "PROT" and resid 64 and name HE1 ))

```

```

ASSI {13271}
(( segid "PROT" and resid 18 and name HN ))
(( segid "PROT" and resid 19 and name HB2 ))
3.400 2.900 2.100 peak 13271 weight 0.10000E+01 volume 0.16318E+01 ppm1 8.476 ppm2 1.409
OR {13271}
(( segid "PROT" and resid 18 and name HN ))
(( segid "PROT" and resid 113 and name HB* ))
ASSI {13881}
(( segid "PROT" and resid 77 and name HN ))
(( segid "PROT" and resid 80 and name HE2 ))
3.600 3.200 1.900 peak 13881 weight 0.10000E+01 volume 0.12199E+01 ppm1 7.383 ppm2 1.915
OR {13881}
(( segid "PROT" and resid 78 and name HN ))
(( segid "PROT" and resid 80 and name HB2 ))
OR {13881}
(( segid "PROT" and resid 77 and name HN ))
(( segid "PROT" and resid 54 and name HG2 ))
OR {13881}
(( segid "PROT" and resid 77 and name HN ))
(( segid "PROT" and resid 73 and name HB2 ))
OR {13881}
(( segid "PROT" and resid 78 and name HN ))
(( segid "PROT" and resid 59 and name HB2 ))
OR {13881}
(( segid "PROT" and resid 78 and name HN ))
(( segid "PROT" and resid 54 and name HG2 ))
ASSI {13971}
(( segid "PROT" and resid 85 and name HN ))
(( segid "PROT" and resid 80 and name HA ))
3.700 3.400 1.800 peak 13971 weight 0.10000E+01 volume 0.93300E+00 ppm1 6.905 ppm2 4.080
OR {13971}
(( segid "PROT" and resid 85 and name HN ))
(( segid "PROT" and resid 53 and name HA ))
ASSI {4172}
(( segid "PROT" and resid 64 and name HE1 ))
(( segid "PROT" and resid 61 and name HG2 ))
2.800 2.000 2.000 peak 4172 weight 0.10000E+01 volume 0.22580E+01 ppm1 3.048 ppm2 2.282
OR {4172}
(( segid "PROT" and resid 97 and name HE1 ))
(( segid "PROT" and resid 94 and name HG1 ))
OR {4172}
(( segid "PROT" and resid 64 and name HE1 ))
(( segid "PROT" and resid 61 and name HB1 ))
ASSI {4232}
(( segid "PROT" and resid 19 and name HE1 ))
(( segid "PROT" and resid 63 and name HD2 ))
2.900 2.100 2.100 peak 4232 weight 0.10000E+01 volume 0.16859E+01 ppm1 3.002 ppm2 1.094
OR {4232}
(( segid "PROT" and resid 19 and name HE1 ))
(( segid "PROT" and resid 22 and name HD1 ))
OR {4232}
(( segid "PROT" and resid 64 and name HE1 ))
(( segid "PROT" and resid 22 and name HD1 ))
ASSI {4242}
(( segid "PROT" and resid 97 and name HE1 ))
(( segid "PROT" and resid 101 and name HD1 ))
2.700 1.800 1.800 peak 4242 weight 0.10000E+01 volume 0.24492E+01 ppm1 3.006 ppm2 0.997
OR {4242}
(( segid "PROT" and resid 6 and name HE1 ))
(( segid "PROT" and resid 116 and name HG12 ))
ASSI {4582}
(( segid "PROT" and resid 86 and name HE1 ))
(( segid "PROT" and resid 99 and name HA ))
2.900 2.100 2.100 peak 4582 weight 0.10000E+01 volume 0.15734E+01 ppm1 2.513 ppm2 3.899
OR {4582}
(( segid "PROT" and resid 86 and name HE1 ))
(( segid "PROT" and resid 83 and name HA ))
ASSI {6142}
(( segid "PROT" and resid 94 and name HG1 ))
(( segid "PROT" and resid 97 and name HE1 ))
2.900 2.100 2.100 peak 6142 weight 0.10000E+01 volume 0.16943E+01 ppm1 2.228 ppm2 3.037
OR {6142}
(( segid "PROT" and resid 87 and name HG2 ))
(( segid "PROT" and resid 84 and name HB1 ))
ASSI {7022}
(( segid "PROT" and resid 64 and name HB1 ))
(( segid "PROT" and resid 61 and name HG1 ))
1.900 1.900 2.600 peak 7022 weight 0.10000E+01 volume 0.22077E+02 ppm1 2.025 ppm2 2.387
OR {7022}
(( segid "PROT" and resid 64 and name HB1 ))
(( segid "PROT" and resid 63 and name HB1 ))
OR {7022}
(( segid "PROT" and resid 39 and name HB1 ))
(( segid "PROT" and resid 42 and name HG1 ))
ASSI {7822}
(( segid "PROT" and resid 97 and name HD1 ))
(( segid "PROT" and resid 94 and name HG1 ))
2.600 1.700 1.700 peak 7822 weight 0.10000E+01 volume 0.31606E+01 ppm1 1.844 ppm2 2.284
OR {7822}

```



```

(( segid "PROT" and resid 97 and name HD1 ))
(( segid "PROT" and resid 92 and name HG2 ))
ASSI { 8232}
(( segid "PROT" and resid 6 and name HD1 ))
(( segid "PROT" and resid 116 and name HD1% ))
2.900 2.100 2.100 peak 8232 weight 0.10000E+01 volume 0.18699E+01 ppm1 1.677 ppm2 0.840
OR { 8232}
(( segid "PROT" and resid 118 and name HD1 ))
(( segid "PROT" and resid 116 and name HG2% ))
OR { 8232}
(( segid "PROT" and resid 6 and name HD1 ))
(( segid "PROT" and resid 116 and name HG2% ))
OR { 8232}
(( segid "PROT" and resid 111 and name HD1 ))
(( segid "PROT" and resid 116 and name HG2% ))
ASSI { 9772}
(( segid "PROT" and resid 110 and name HG12 ))
(( segid "PROT" and resid 115 and name HB2 ))
3.000 2.200 2.200 peak 9772 weight 0.10000E+01 volume 0.15374E+01 ppm1 1.125 ppm2 1.618
OR { 9772}
(( segid "PROT" and resid 110 and name HG11 ))
(( segid "PROT" and resid 115 and name HB2 ))
OR { 9772}
(( segid "PROT" and resid 110 and name HG11 ))
(( segid "PROT" and resid 109 and name HB2 ))
ASSI { 9822}
(( segid "PROT" and resid 78 and name HD1% ))
(( segid "PROT" and resid 74 and name HD% ))
2.400 1.400 1.400 peak 9822 weight 0.10000E+01 volume 0.47381E+01 ppm1 0.096 ppm2 6.459
OR { 9822}
(( segid "PROT" and resid 78 and name HD1% ))
(( segid "PROT" and resid 82 and name HE% ))
ASSI { 9952}
(( segid "PROT" and resid 97 and name HG2 ))
(( segid "PROT" and resid 94 and name HA ))
2.400 1.400 1.400 peak 9952 weight 0.10000E+01 volume 0.50570E+01 ppm1 1.607 ppm2 4.239
OR { 9952}
(( segid "PROT" and resid 97 and name HG2 ))
(( segid "PROT" and resid 97 and name HA ))
ASSI {10652}
(( segid "PROT" and resid 6 and name HG1 ))
(( segid "PROT" and resid 115 and name HA ))
2.400 1.400 1.400 peak 10652 weight 0.10000E+01 volume 0.48739E+01 ppm1 1.470 ppm2 4.248
OR {10652}
(( segid "PROT" and resid 6 and name HG1 ))
(( segid "PROT" and resid 116 and name HA ))
OR {10652}
(( segid "PROT" and resid 6 and name HG2 ))
(( segid "PROT" and resid 115 and name HA ))
OR {10652}
(( segid "PROT" and resid 6 and name HG2 ))
(( segid "PROT" and resid 116 and name HA ))
OR {10652}
(( segid "PROT" and resid 111 and name HG1 ))
(( segid "PROT" and resid 108 and name HA ))
ASSI {10712}
(( segid "PROT" and resid 57 and name HG1 ))
(( segid "PROT" and resid 37 and name HB1 ))
2.500 1.600 1.600 peak 10712 weight 0.10000E+01 volume 0.40188E+01 ppm1 1.522 ppm2 2.399
OR {10712}
(( segid "PROT" and resid 57 and name HG1 ))
(( segid "PROT" and resid 55 and name HB1 ))
ASSI {10852}
(( segid "PROT" and resid 6 and name HG2 ))
(( segid "PROT" and resid 6 and name HD1 ))
1.600 0.600 0.600 peak 10852 weight 0.10000E+01 volume 0.64288E+02 ppm1 1.461 ppm2 1.709
OR {10852}
(( segid "PROT" and resid 104 and name HG2 ))
(( segid "PROT" and resid 104 and name HD1 ))
OR {10852}
(( segid "PROT" and resid 6 and name HG1 ))
(( segid "PROT" and resid 6 and name HD1 ))
ASSI {11042}
(( segid "PROT" and resid 102 and name HD2% ))
(( segid "PROT" and resid 28 and name HA ))
2.600 1.700 1.700 peak 11042 weight 0.10000E+01 volume 0.30164E+01 ppm1 0.766 ppm2 3.994
OR {11042}
(( segid "PROT" and resid 102 and name HD2% ))
(( segid "PROT" and resid 30 and name HB2 ))
OR {11042}
(( segid "PROT" and resid 102 and name HD2% ))
(( segid "PROT" and resid 106 and name HA ))
ASSI {11372}
(( segid "PROT" and resid 115 and name HD2% ))
(( segid "PROT" and resid 75 and name HE% ))
2.800 2.000 2.000 peak 11372 weight 0.10000E+01 volume 0.22403E+01 ppm1 0.792 ppm2 2.095
OR {11372}
(( segid "PROT" and resid 115 and name HD2% ))
(( segid "PROT" and resid 8 and name HG1 ))

```

```

ASSI {11542}
( segid "PROT" and resid 25 and name HG1% )
( segid "PROT" and resid 31 and name HB% )
2.800 2.000 2.000 peak 11542 weight 0.10000E+01 volume 0.19754E+01 ppm1 1.246 ppm2 1.764
OR {11542}
( segid "PROT" and resid 25 and name HG1% )
(( segid "PROT" and resid 21 and name HG11 ))
OR {11542}
( segid "PROT" and resid 25 and name HG1% )
(( segid "PROT" and resid 22 and name HB2 ))
OR {11542}
( segid "PROT" and resid 25 and name HG1% )
(( segid "PROT" and resid 22 and name HG ))
ASSI {11582}
( segid "PROT" and resid 25 and name HG1% )
( segid "PROT" and resid 56 and name HD2% )
2.700 1.800 1.800 peak 11582 weight 0.10000E+01 volume 0.27149E+01 ppm1 1.242 ppm2 0.676
OR {11582}
( segid "PROT" and resid 25 and name HG1% )
(( segid "PROT" and resid 78 and name HG ))
OR {11582}
( segid "PROT" and resid 25 and name HG1% )
( segid "PROT" and resid 110 and name HG2% )
ASSI {11652}
( segid "PROT" and resid 83 and name HG2% )
(( segid "PROT" and resid 86 and name HB1 ))
2.800 2.000 2.000 peak 11652 weight 0.10000E+01 volume 0.20985E+01 ppm1 1.322 ppm2 1.811
OR {11652}
( segid "PROT" and resid 83 and name HG2% )
(( segid "PROT" and resid 80 and name HG1 ))
OR {11652}
( segid "PROT" and resid 41 and name HG2% )
(( segid "PEPT" and resid 208 and name HB1 ))
ASSI {11842}
( segid "PROT" and resid 81 and name HG1% )
(( segid "PROT" and resid 56 and name HG ))
2.900 2.100 2.100 peak 11842 weight 0.10000E+01 volume 0.17306E+01 ppm1 0.514 ppm2 1.778
OR {11842}
( segid "PROT" and resid 81 and name HG1% )
(( segid "PROT" and resid 80 and name HG1 ))
OR {11842}
( segid "PROT" and resid 38 and name HG1% )
(( segid "PEPT" and resid 205 and name HB1 ))
OR {11842}
( segid "PROT" and resid 38 and name HG1% )
(( segid "PROT" and resid 36 and name HB2 ))
ASSI {12152}
( segid "PROT" and resid 69 and name HG1% )
(( segid "PROT" and resid 11 and name HB2 ))
2.900 2.100 2.100 peak 12152 weight 0.10000E+01 volume 0.15613E+01 ppm1 0.986 ppm2 2.048
OR {12152}
( segid "PROT" and resid 69 and name HG1% )
(( segid "PROT" and resid 66 and name HB2 ))
ASSI {12162}
( segid "PROT" and resid 17 and name HG2% )
(( segid "PROT" and resid 115 and name HG ))
2.700 1.800 1.800 peak 12162 weight 0.10000E+01 volume 0.25853E+01 ppm1 1.176 ppm2 1.577
OR {12162}
( segid "PROT" and resid 17 and name HG2% )
(( segid "PROT" and resid 109 and name HB2 ))
ASSI {12662}
( segid "PROT" and resid 113 and name HB% )
(( segid "PROT" and resid 110 and name HB ))
2.600 1.700 1.700 peak 12662 weight 0.10000E+01 volume 0.30533E+01 ppm1 1.409 ppm2 1.786
OR {12662}
( segid "PROT" and resid 113 and name HB% )
(( segid "PROT" and resid 109 and name HB1 ))
OR {12662}
( segid "PROT" and resid 113 and name HB% )
(( segid "PROT" and resid 21 and name HG11 ))
ASSI {12692}
( segid "PROT" and resid 113 and name HB% )
(( segid "PROT" and resid 21 and name HG12 ))
2.900 2.100 2.100 peak 12692 weight 0.10000E+01 volume 0.17007E+01 ppm1 1.416 ppm2 1.073
OR {12692}
( segid "PROT" and resid 113 and name HB% )
(( segid "PROT" and resid 110 and name HG12 ))
ASSI {13152}
( segid "PROT" and resid 21 and name HG2% )
(( segid "PROT" and resid 24 and name HG2 ))
2.900 2.100 2.100 peak 13152 weight 0.10000E+01 volume 0.16396E+01 ppm1 1.019 ppm2 2.511
OR {13152}
( segid "PROT" and resid 21 and name HG2% )
(( segid "PROT" and resid 109 and name HE2 ))
ASSI {13172}
( segid "PROT" and resid 21 and name HG2% )
( segid "PROT" and resid 113 and name HB% )
2.900 2.100 2.100 peak 13172 weight 0.10000E+01 volume 0.15888E+01 ppm1 1.022 ppm2 1.412
OR {13172}

```

```

( segid "PROT" and resid 21 and name HG2%)
(( segid "PROT" and resid 109 and name HD1 ))
ASSI {13282}
( segid "PROT" and resid 75 and name HE% )
(( segid "PROT" and resid 6 and name HE1 ))
2.700 1.800 1.800 peak 13282 weight 0.10000E+01 volume 0.29048E+01 ppm1 2.097 ppm2 3.036
OR {13282}
( segid "PROT" and resid 75 and name HE% )
(( segid "PROT" and resid 74 and name HB1 ))
OR {13282}
( segid "PROT" and resid 75 and name HE% )
(( segid "PROT" and resid 82 and name HB2 ))
ASSI {13352}
( segid "PROT" and resid 75 and name HE% )
( segid "PROT" and resid 113 and name HB% )
2.900 2.100 2.100 peak 13352 weight 0.10000E+01 volume 0.15571E+01 ppm1 2.095 ppm2 1.436
OR {13352}
( segid "PROT" and resid 75 and name HE% )
(( segid "PROT" and resid 6 and name HG1 ))
OR {13352}
( segid "PROT" and resid 75 and name HE% )
(( segid "PROT" and resid 6 and name HG2 ))
OR {13352}
( segid "PROT" and resid 75 and name HE% )
(( segid "PROT" and resid 81 and name HB ))
ASSI {14022}
( segid "PROT" and resid 116 and name HD1%)
(( segid "PROT" and resid 107 and name HA ))
2.900 2.100 2.100 peak 14022 weight 0.10000E+01 volume 0.16161E+01 ppm1 0.826 ppm2 3.863
OR {14022}
( segid "PROT" and resid 116 and name HD1%)
(( segid "PROT" and resid 110 and name HA ))
ASSI {14402}
(( segid "PROT" and resid 74 and name HB2 ))
(( segid "PROT" and resid 75 and name HA ))
3.200 2.600 2.300 peak 14402 weight 0.10000E+01 volume 0.10054E+01 ppm1 2.415 ppm2 4.066
OR {14402}
(( segid "PROT" and resid 74 and name HB2 ))
(( segid "PROT" and resid 15 and name HA ))
OR {14402}
(( segid "PROT" and resid 74 and name HB2 ))
(( segid "PROT" and resid 72 and name HA ))
ASSI {14792}
(( segid "PROT" and resid 53 and name HG1 ))
(( segid "PROT" and resid 52 and name HB1 ))
3.300 2.700 2.200 peak 14792 weight 0.10000E+01 volume 0.77210E+00 ppm1 2.267 ppm2 3.049
OR {14792}
(( segid "PROT" and resid 53 and name HG1 ))
(( segid "PROT" and resid 84 and name HB1 ))
ASSI {15152}
(( segid "PROT" and resid 96 and name HB1 ))
( segid "PROT" and resid 99 and name HB% )
3.200 2.600 2.300 peak 15152 weight 0.10000E+01 volume 0.91940E+00 ppm1 3.417 ppm2 1.640
OR {15152}
(( segid "PROT" and resid 96 and name HB1 ))
(( segid "PROT" and resid 97 and name HG2 ))
ASSI {15342}
( segid "PROT" and resid 38 and name HG2%)
(( segid "PROT" and resid 53 and name HA ))
3.200 2.600 2.300 peak 15342 weight 0.10000E+01 volume 0.94230E+00 ppm1 -0.005 ppm2 4.101
OR {15342}
( segid "PROT" and resid 38 and name HG2%)
(( segid "PROT" and resid 41 and name HA ))
ASSI {15372}
( segid "PROT" and resid 38 and name HG2%)
(( segid "PROT" and resid 46 and name HB2 ))
3.000 2.200 2.200 peak 15372 weight 0.10000E+01 volume 0.13687E+01 ppm1 -0.009 ppm2 2.414
OR {15372}
( segid "PROT" and resid 38 and name HG2%)
(( segid "PROT" and resid 37 and name HB1 ))
ASSI {15382}
( segid "PROT" and resid 38 and name HG2%)
(( segid "PROT" and resid 39 and name HB2 ))
3.000 2.200 2.200 peak 15382 weight 0.10000E+01 volume 0.12723E+01 ppm1 -0.012 ppm2 1.942
OR {15382}
( segid "PROT" and resid 38 and name HG2%)
(( segid "PROT" and resid 53 and name HG2 ))
ASSI {15422}
( segid "PROT" and resid 81 and name HG2%)
(( segid "PROT" and resid 80 and name HB2 ))
3.200 2.600 2.300 peak 15422 weight 0.10000E+01 volume 0.98300E+00 ppm1 0.152 ppm2 1.938
OR {15422}
( segid "PROT" and resid 81 and name HG2%)
(( segid "PROT" and resid 59 and name HB2 ))
ASSI {15442}
( segid "PROT" and resid 81 and name HG2%)
(( segid "PROT" and resid 31 and name HA ))
3.200 2.600 2.300 peak 15442 weight 0.10000E+01 volume 0.91520E+00 ppm1 0.154 ppm2 4.431
OR {15442}

```

```

( segid "PROT" and resid 81 and name HG2%)
(( segid "PROT" and resid 77 and name HA ))
ASSI {15682}
( segid "PROT" and resid 18 and name HD2%)
(( segid "PROT" and resid 74 and name HA ))
3.300 2.700 2.200 peak 15682 weight 0.10000E+01 volume 0.81490E+00 ppm1 -0.161 ppm2 3.801
OR {15682}
( segid "PROT" and resid 18 and name HD2%)
(( segid "PROT" and resid 70 and name HB2 ))
ASSI {16372}
( segid "PROT" and resid 78 and name HD2%)
(( segid "PROT" and resid 22 and name HA ))
3.200 2.600 2.300 peak 16372 weight 0.10000E+01 volume 0.10279E+01 ppm1 0.201 ppm2 4.142
OR {16372}
(( segid "PROT" and resid 50 and name HG12%))
(( segid "PROT" and resid 53 and name HA ))
OR {16372}
(( segid "PROT" and resid 50 and name HG12%))
(( segid "PROT" and resid 47 and name HA ))
ASSI {16562}
(( segid "PROT" and resid 115 and name HB2 ))
(( segid "PROT" and resid 110 and name HG11%))
3.200 2.600 2.300 peak 16562 weight 0.10000E+01 volume 0.10189E+01 ppm1 1.619 ppm2 1.169
OR {16562}
(( segid "PROT" and resid 115 and name HB2 ))
( segid "PROT" and resid 17 and name HG2%)
ASSI {16752}
( segid "PROT" and resid 21 and name HD1%)
(( segid "PROT" and resid 20 and name HB1 ))
3.100 2.400 2.400 peak 16752 weight 0.10000E+01 volume 0.11661E+01 ppm1 0.657 ppm2 4.106
OR {16752}
( segid "PROT" and resid 21 and name HD1%)
(( segid "PROT" and resid 109 and name HA ))
ASSI {16872}
( segid "PROT" and resid 78 and name HD2%)
(( segid "PROT" and resid 56 and name HG ))
3.300 2.700 2.200 peak 16872 weight 0.10000E+01 volume 0.83710E+00 ppm1 0.182 ppm2 1.768
OR {16872}
( segid "PROT" and resid 78 and name HD2%)
( segid "PROT" and resid 31 and name HB% )
OR {16872}
( segid "PROT" and resid 78 and name HD2%)
(( segid "PROT" and resid 22 and name HG ))
OR {16872}
( segid "PROT" and resid 78 and name HD2%)
(( segid "PROT" and resid 22 and name HB2 ))
ASSI {16942}
( segid "PROT" and resid 50 and name HG2%)
( segid "PROT" and resid 49 and name HG2%)
3.200 2.600 2.300 peak 16942 weight 0.10000E+01 volume 0.10136E+01 ppm1 0.420 ppm2 0.947
OR {16942}
( segid "PROT" and resid 50 and name HG2%)
( segid "PROT" and resid 43 and name HB% )
ASSI {17202}
( segid "PROT" and resid 110 and name HG2%)
(( segid "PROT" and resid 75 and name HB2 ))
3.400 2.900 2.100 peak 17202 weight 0.10000E+01 volume 0.64990E+00 ppm1 0.697 ppm2 2.651
OR {17202}
( segid "PROT" and resid 110 and name HG2%)
(( segid "PROT" and resid 109 and name HE1 ))
ASSI {17212}
( segid "PROT" and resid 110 and name HG2%)
(( segid "PROT" and resid 75 and name HA ))
3.000 2.200 2.200 peak 17212 weight 0.10000E+01 volume 0.13418E+01 ppm1 0.693 ppm2 4.096
OR {17212}
( segid "PROT" and resid 110 and name HG2%)
(( segid "PROT" and resid 109 and name HA ))
OR {17212}
( segid "PROT" and resid 110 and name HG2%)
(( segid "PROT" and resid 111 and name HA ))
ASSI {17222}
( segid "PROT" and resid 110 and name HG2%)
(( segid "PROT" and resid 115 and name HA ))
3.000 2.200 2.200 peak 17222 weight 0.10000E+01 volume 0.12816E+01 ppm1 0.693 ppm2 4.268
OR {17222}
( segid "PROT" and resid 110 and name HG2%)
(( segid "PROT" and resid 17 and name HB ))
OR {17222}
( segid "PROT" and resid 110 and name HG2%)
(( segid "PROT" and resid 116 and name HA ))
OR {17222}
( segid "PROT" and resid 110 and name HG2%)
(( segid "PROT" and resid 108 and name HA ))
ASSI {17242}
( segid "PROT" and resid 110 and name HD1%)
(( segid "PROT" and resid 75 and name HB1 ))
3.200 2.600 2.300 peak 17242 weight 0.10000E+01 volume 0.96060E+00 ppm1 0.566 ppm2 2.968
OR {17242}
( segid "PROT" and resid 110 and name HD1%)

```

```

(( segid "PROT" and resid 74 and name HB1 ))
ASSI {17732}
(( segid "PROT" and resid 104 and name HB1 ))
(( segid "PROT" and resid 105 and name HB2 ))
3.000 2.200 2.200 peak 17732 weight 0.10000E+01 volume 0.13380E+01 ppm1 1.956 ppm2 3.093
OR {17732}
(( segid "PROT" and resid 104 and name HB1 ))
(( segid "PROT" and resid 107 and name HB1 ))
ASSI {18402}
(( segid "PROT" and resid 54 and name HE% ))
(( segid "PROT" and resid 78 and name HA ))
3.200 2.600 2.300 peak 18402 weight 0.10000E+01 volume 0.91630E+00 ppm1 2.004 ppm2 3.407
OR {18402}
(( segid "PROT" and resid 54 and name HE% ))
(( segid "PROT" and resid 53 and name HD2 ))
OR {18402}
(( segid "PROT" and resid 54 and name HE% ))
(( segid "PROT" and resid 80 and name HD1 ))
ASSI {18632}
(( segid "PROT" and resid 75 and name HE% ))
(( segid "PROT" and resid 107 and name HA ))
3.200 2.600 2.300 peak 18632 weight 0.10000E+01 volume 0.93700E+00 ppm1 2.094 ppm2 3.856
OR {18632}
(( segid "PROT" and resid 75 and name HE% ))
(( segid "PROT" and resid 79 and name HA ))
ASSI {19102}
(( segid "PROT" and resid 52 and name HB2 ))
(( segid "PROT" and resid 80 and name HG1 ))
3.300 2.700 2.200 peak 19102 weight 0.10000E+01 volume 0.80800E+00 ppm1 2.952 ppm2 1.789
OR {19102}
(( segid "PROT" and resid 100 and name HB1 ))
(( segid "PROT" and resid 103 and name HB1 ))
OR {19102}
(( segid "PROT" and resid 100 and name HB1 ))
(( segid "PROT" and resid 97 and name HG1 ))
ASSI {19112}
(( segid "PROT" and resid 52 and name HB2 ))
(( segid "PROT" and resid 80 and name HB2 ))
3.300 2.700 2.200 peak 19112 weight 0.10000E+01 volume 0.85230E+00 ppm1 2.952 ppm2 1.953
OR {19112}
(( segid "PROT" and resid 100 and name HB1 ))
(( segid "PROT" and resid 101 and name HB ))
ASSI {19132}
(( segid "PROT" and resid 19 and name HB2 ))
(( segid "PROT" and resid 63 and name HD2% ))
3.100 2.400 2.400 peak 19132 weight 0.10000E+01 volume 0.11757E+01 ppm1 1.414 ppm2 1.074
OR {19132}
(( segid "PROT" and resid 19 and name HB2 ))
(( segid "PROT" and resid 22 and name HD1% ))
ASSI {19302}
(( segid "PROT" and resid 97 and name HG1 ))
(( segid "PROT" and resid 94 and name HA ))
2.500 1.600 1.600 peak 19302 weight 0.10000E+01 volume 0.38386E+01 ppm1 1.850 ppm2 4.236
OR {19302}
(( segid "PROT" and resid 97 and name HG1 ))
(( segid "PROT" and resid 97 and name HA ))
ASSI {19402}
(( segid "PROT" and resid 49 and name HG1% ))
(( segid "PROT" and resid 84 and name HB1 ))
2.900 2.100 2.100 peak 19402 weight 0.10000E+01 volume 0.15644E+01 ppm1 0.969 ppm2 3.045
OR {19402}
(( segid "PROT" and resid 43 and name HB% ))
(( segid "PEPT" and resid 205 and name HE1 ))
ASSI {19792}
(( segid "PROT" and resid 25 and name HG2% ))
(( segid "PROT" and resid 56 and name HB2 ))
3.000 2.200 2.200 peak 19792 weight 0.10000E+01 volume 0.14304E+01 ppm1 1.076 ppm2 1.466
OR {19792}
(( segid "PROT" and resid 25 and name HG2% ))
(( segid "PROT" and resid 102 and name HB1 ))
ASSI {19832}
(( segid "PROT" and resid 58 and name HG2% ))
(( segid "PROT" and resid 57 and name HE1 ))
2.600 1.700 1.700 peak 19832 weight 0.10000E+01 volume 0.33967E+01 ppm1 1.097 ppm2 2.611
OR {19832}
(( segid "PROT" and resid 25 and name HG2% ))
(( segid "PROT" and resid 34 and name HB2 ))
ASSI {19842}
(( segid "PROT" and resid 58 and name HG2% ))
(( segid "PROT" and resid 61 and name HG2 ))
3.100 2.400 2.400 peak 19842 weight 0.10000E+01 volume 0.11239E+01 ppm1 1.100 ppm2 2.265
OR {19842}
(( segid "PROT" and resid 58 and name HG2% ))
(( segid "PROT" and resid 61 and name HB1 ))
OR {19842}
(( segid "PROT" and resid 58 and name HG2% ))
(( segid "PROT" and resid 53 and name HB1 ))
ASSI {20142}
(( segid "PROT" and resid 39 and name HB2 ))

```

```

( segid "PROT" and resid 38 and name HG1% )
3.500 3.100 2.000 peak 20142 weight 0.10000E+01 volume 0.60320E+00 ppm1 1.913 ppm2 0.516
OR {20142}
(( segid "PROT" and resid 8 and name HB2 ))
(( segid "PROT" and resid 18 and name HD1% ))
ASSI {20192}
( segid "PROT" and resid 102 and name HD1% )
(( segid "PROT" and resid 28 and name HB1 ))
2.800 2.000 2.000 peak 20192 weight 0.10000E+01 volume 0.20545E+01 ppm1 0.754 ppm2 3.007
OR {20192}
( segid "PROT" and resid 115 and name HD1% )
(( segid "PROT" and resid 74 and name HB1 ))
ASSI {21012}
( segid "PROT" and resid 35 and name HE% )
( segid "PROT" and resid 25 and name HG2% )
3.300 2.700 2.200 peak 21012 weight 0.10000E+01 volume 0.73890E+00 ppm1 2.221 ppm2 1.062
OR {21012}
( segid "PROT" and resid 35 and name HE% )
( segid "PROT" and resid 22 and name HD2% )
ASSI {21052}
( segid "PROT" and resid 50 and name HD1% )
( segid "PROT" and resid 83 and name HG2% )
3.600 3.200 1.900 peak 21052 weight 0.10000E+01 volume 0.47270E+00 ppm1 0.580 ppm2 1.342
OR {21052}
( segid "PROT" and resid 50 and name HD1% )
(( segid "PROT" and resid 51 and name HG1 ))
OR {21052}
( segid "PROT" and resid 50 and name HD1% )
(( segid "PROT" and resid 86 and name HG1 ))
ASSI {21072}
( segid "PROT" and resid 110 and name HD1% )
(( segid "PROT" and resid 107 and name HB1 ))
3.300 2.700 2.200 peak 21072 weight 0.10000E+01 volume 0.77140E+00 ppm1 0.567 ppm2 3.097
OR {21072}
( segid "PROT" and resid 110 and name HD1% )
(( segid "PROT" and resid 106 and name HB2 ))
ASSI {21122}
( segid "PROT" and resid 110 and name HD1% )
(( segid "PROT" and resid 75 and name HA ))
3.300 2.700 2.200 peak 21122 weight 0.10000E+01 volume 0.76390E+00 ppm1 0.564 ppm2 4.090
OR {21122}
( segid "PROT" and resid 110 and name HD1% )
(( segid "PROT" and resid 111 and name HA ))
ASSI {21192}
( segid "PROT" and resid 21 and name HD1% )
(( segid "PROT" and resid 109 and name HE2 ))
3.500 3.100 2.000 peak 21192 weight 0.10000E+01 volume 0.57950E+00 ppm1 0.655 ppm2 2.513
OR {21192}
( segid "PROT" and resid 21 and name HD1% )
(( segid "PROT" and resid 24 and name HG2 ))
ASSI {21202}
( segid "PROT" and resid 101 and name HD1% )
(( segid "PROT" and resid 29 and name HG1 ))
3.300 2.700 2.200 peak 21202 weight 0.10000E+01 volume 0.73140E+00 ppm1 1.003 ppm2 2.491
OR {21202}
( segid "PROT" and resid 101 and name HD1% )
(( segid "PROT" and resid 86 and name HE2 ))
ASSI {21252}
( segid "PROT" and resid 54 and name HE% )
(( segid "PROT" and resid 52 and name HB1 ))
3.300 2.700 2.200 peak 21252 weight 0.10000E+01 volume 0.73170E+00 ppm1 2.001 ppm2 3.055
OR {21252}
( segid "PROT" and resid 54 and name HE% )
(( segid "PROT" and resid 68 and name HB1 ))
ASSI {21262}
( segid "PROT" and resid 59 and name HE% )
(( segid "PROT" and resid 22 and name HG ))
3.300 2.700 2.200 peak 21262 weight 0.10000E+01 volume 0.72600E+00 ppm1 1.304 ppm2 1.770
OR {21262}
( segid "PROT" and resid 59 and name HE% )
(( segid "PROT" and resid 22 and name HB2 ))
OR {21262}
( segid "PROT" and resid 59 and name HE% )
(( segid "PROT" and resid 56 and name HG ))
ASSI {21272}
( segid "PROT" and resid 59 and name HE% )
(( segid "PROT" and resid 74 and name HB2 ))
3.500 3.100 2.000 peak 21272 weight 0.10000E+01 volume 0.59840E+00 ppm1 1.308 ppm2 2.414
OR {21272}
( segid "PROT" and resid 59 and name HE% )
(( segid "PROT" and resid 25 and name HB ))
ASSI {21282}
( segid "PROT" and resid 59 and name HE% )
(( segid "PROT" and resid 68 and name HB2 ))
3.300 2.700 2.200 peak 21282 weight 0.10000E+01 volume 0.76270E+00 ppm1 1.307 ppm2 2.928
OR {21282}
( segid "PROT" and resid 59 and name HE% )
(( segid "PROT" and resid 75 and name HB1 ))
ASSI {21292}

```

```

( segid "PROT" and resid 59 and name HE% )
(( segid "PROT" and resid 74 and name HB1 ))
3.100 2.400 2.400 peak 21292 weight 0.10000E+01 volume 0.12489E+01 ppm1 1.307 ppm2 3.001
OR {21292}
( segid "PROT" and resid 59 and name HE% )
(( segid "PROT" and resid 82 and name HB2 ))
ASSI {21302}
( segid "PROT" and resid 50 and name HG2% )
(( segid "PROT" and resid 81 and name HA ))
3.300 2.700 2.200 peak 21302 weight 0.10000E+01 volume 0.74050E+00 ppm1 0.418 ppm2 3.139
OR {21302}
( segid "PROT" and resid 50 and name HG2% )
(( segid "PROT" and resid 85 and name HB2 ))
ASSI {21392}
( segid "PROT" and resid 75 and name HE% )
(( segid "PROT" and resid 21 and name HG11 ))
2.900 2.100 2.100 peak 21392 weight 0.10000E+01 volume 0.16056E+01 ppm1 2.097 ppm2 1.744
OR {21392}
( segid "PROT" and resid 75 and name HE% )
(( segid "PROT" and resid 109 and name HB1 ))
ASSI {21422}
( segid "PROT" and resid 75 and name HE% )
( segid "PROT" and resid 106 and name HD% )
3.400 2.900 2.100 peak 21422 weight 0.10000E+01 volume 0.65170E+00 ppm1 2.094 ppm2 6.965
OR {21422}
( segid "PROT" and resid 75 and name HE% )
( segid "PROT" and resid 74 and name HE% )
ASSI {21532}
( segid "PROT" and resid 101 and name HG2% )
(( segid "PROT" and resid 29 and name HG1 ))
3.100 2.400 2.400 peak 21532 weight 0.10000E+01 volume 0.11597E+01 ppm1 1.029 ppm2 2.512
OR {21532}
( segid "PROT" and resid 101 and name HG2% )
(( segid "PROT" and resid 24 and name HB1 ))
ASSI {21542}
( segid "PROT" and resid 101 and name HG2% )
(( segid "PROT" and resid 28 and name HB1 ))
3.000 2.200 2.200 peak 21542 weight 0.10000E+01 volume 0.12716E+01 ppm1 1.029 ppm2 3.048
OR {21542}
( segid "PROT" and resid 101 and name HG2% )
(( segid "PROT" and resid 98 and name HB2 ))
OR {21542}
( segid "PROT" and resid 101 and name HG2% )
(( segid "PROT" and resid 104 and name HB1 ))
ASSI {21652}
( segid "PROT" and resid 99 and name HB% )
(( segid "PROT" and resid 101 and name HB ))
3.200 2.600 2.300 peak 21652 weight 0.10000E+01 volume 0.91970E+00 ppm1 1.661 ppm2 1.940
OR {21652}
( segid "PROT" and resid 99 and name HB% )
(( segid "PROT" and resid 103 and name HG2 ))
ASSI {21882}
( segid "PROT" and resid 113 and name HB% )
(( segid "PROT" and resid 112 and name HG2 ))
3.600 3.200 1.900 peak 21882 weight 0.10000E+01 volume 0.47230E+00 ppm1 1.410 ppm2 2.255
OR {21882}
( segid "PROT" and resid 113 and name HB% )
(( segid "PROT" and resid 75 and name HG2 ))
ASSI {21912}
( segid "PROT" and resid 113 and name HB% )
(( segid "PROT" and resid 112 and name HA ))
3.100 2.400 2.400 peak 21912 weight 0.10000E+01 volume 0.12419E+01 ppm1 1.406 ppm2 4.025
OR {21912}
( segid "PROT" and resid 113 and name HB% )
(( segid "PROT" and resid 106 and name HA ))
ASSI {21932}
( segid "PROT" and resid 18 and name HD2% )
( segid "PROT" and resid 21 and name HG2% )
3.100 2.400 2.400 peak 21932 weight 0.10000E+01 volume 0.10470E+01 ppm1 -0.162 ppm2 1.023
OR {21932}
( segid "PROT" and resid 18 and name HD2% )
( segid "PROT" and resid 22 and name HD2% )
ASSI {21942}
( segid "PROT" and resid 18 and name HD2% )
( segid "PROT" and resid 113 and name HB% )
3.400 2.900 2.100 peak 21942 weight 0.10000E+01 volume 0.65970E+00 ppm1 -0.162 ppm2 1.424
OR {21942}
( segid "PROT" and resid 18 and name HD2% )
(( segid "PROT" and resid 14 and name HG ))
ASSI {22002}
( segid "PROT" and resid 43 and name HB% )
(( segid "PROT" and resid 39 and name HA ))
3.300 2.700 2.200 peak 22002 weight 0.10000E+01 volume 0.79200E+00 ppm1 0.988 ppm2 4.446
OR {22002}
( segid "PROT" and resid 43 and name HB% )
(( segid "PEPT" and resid 204 and name HA ))
ASSI {22012}
( segid "PROT" and resid 49 and name HG2% )
(( segid "PROT" and resid 87 and name HB2 ))

```

```

3.100      2.400      2.400 peak 22012 weight 0.10000E+01 volume 0.12017E+01 ppm1 0.909 ppm2 2.082
OR {22012}
( segid "PROT" and resid 49 and name HG2%)
(( segid "PROT" and resid 48 and name HB2 ))
ASSI {22162}
( segid "PROT" and resid 25 and name HG2%)
(( segid "PROT" and resid 31 and name HA ))
3.300      2.700      2.200 peak 22162 weight 0.10000E+01 volume 0.83230E+00 ppm1 1.084 ppm2 4.438
OR {22162}
( segid "PROT" and resid 25 and name HG2%)
(( segid "PROT" and resid 60 and name HA ))
ASSI {22242}
( segid "PROT" and resid 115 and name HD2%)
(( segid "PROT" and resid 21 and name HG11))
2.200      2.200      2.300 peak 22242 weight 0.10000E+01 volume 0.90954E+01 ppm1 0.786 ppm2 1.755
OR {22242}
( segid "PROT" and resid 115 and name HD2%)
(( segid "PROT" and resid 109 and name HB1 ))
OR {22242}
( segid "PROT" and resid 115 and name HD2%)
(( segid "PROT" and resid 111 and name HB2 ))
ASSI {22252}
( segid "PROT" and resid 115 and name HD2%)
(( segid "PROT" and resid 75 and name HG2 ))
3.200      2.600      2.300 peak 22252 weight 0.10000E+01 volume 0.10049E+01 ppm1 0.783 ppm2 2.265
OR {22252}
( segid "PROT" and resid 115 and name HD2%)
(( segid "PROT" and resid 8 and name HB1 ))
ASSI {22272}
( segid "PROT" and resid 73 and name HD2%)
(( segid "PROT" and resid 74 and name HB1 ))
3.200      2.600      2.300 peak 22272 weight 0.10000E+01 volume 0.88380E+00 ppm1 0.924 ppm2 3.008
OR {22272}
( segid "PROT" and resid 73 and name HD2%)
(( segid "PROT" and resid 67 and name HB1 ))
ASSI {22332}
( segid "PROT" and resid 22 and name HD2%)
(( segid "PROT" and resid 59 and name HA ))
3.200      2.600      2.300 peak 22332 weight 0.10000E+01 volume 0.10249E+01 ppm1 1.047 ppm2 4.341
OR {22332}
( segid "PROT" and resid 22 and name HD2%)
(( segid "PROT" and resid 35 and name HA ))
OR {22332}
( segid "PROT" and resid 22 and name HD2%)
(( segid "PROT" and resid 20 and name HA ))
ASSI {22372}
( segid "PROT" and resid 78 and name HD2%)
(( segid "PROT" and resid 25 and name HB ))
3.600      3.200      1.900 peak 22372 weight 0.10000E+01 volume 0.49530E+00 ppm1 0.195 ppm2 2.453
OR {22372}
( segid "PROT" and resid 78 and name HD2%)
(( segid "PROT" and resid 74 and name HB2 ))
ASSI {22392}
( segid "PROT" and resid 102 and name HD2%)
( segid "PROT" and resid 35 and name HB )
3.700      3.400      1.800 peak 22392 weight 0.10000E+01 volume 0.42720E+00 ppm1 0.760 ppm2 2.234
OR {22392}
( segid "PROT" and resid 102 and name HD2%)
(( segid "PROT" and resid 33 and name HD1 ))
OR {22392}
( segid "PROT" and resid 102 and name HD2%)
(( segid "PROT" and resid 35 and name HB2 ))
ASSI {22412}
( segid "PROT" and resid 78 and name HD2%)
(( segid "PROT" and resid 77 and name HB1 ))
3.600      3.200      1.900 peak 22412 weight 0.10000E+01 volume 0.45250E+00 ppm1 0.190 ppm2 2.741
OR {22412}
(( segid "PROT" and resid 50 and name HG12))
(( segid "PROT" and resid 84 and name HB2 ))
ASSI {22442}
( segid "PROT" and resid 102 and name HD2%)
(( segid "PROT" and resid 98 and name HB1 ))
3.600      3.200      1.900 peak 22442 weight 0.10000E+01 volume 0.48990E+00 ppm1 0.759 ppm2 3.407
OR {22442}
( segid "PROT" and resid 102 and name HD2%)
(( segid "PROT" and resid 78 and name HA ))
ASSI {22452}
( segid "PROT" and resid 78 and name HD2%)
(( segid "PROT" and resid 56 and name HA ))
3.400      2.900      2.100 peak 22452 weight 0.10000E+01 volume 0.69950E+00 ppm1 0.201 ppm2 4.065
OR {22452}
( segid "PROT" and resid 78 and name HD2%)
(( segid "PROT" and resid 75 and name HA ))
ASSI {22462}
( segid "PROT" and resid 78 and name HD2%)
(( segid "PROT" and resid 79 and name HA ))
3.200      2.600      2.300 peak 22462 weight 0.10000E+01 volume 0.93720E+00 ppm1 0.203 ppm2 3.868
OR {22462}
( segid "PROT" and resid 78 and name HD2%)

```



```

(( segid "PROT" and resid 25 and name HA ))
ASSI {22532}
( segid "PROT" and resid 78 and name HD2%)
( segid "PROT" and resid 34 and name HD% )
3.400 2.900 2.100 peak 22532 weight 0.10000E+01 volume 0.68350E+00 ppm1 0 199 ppm2 7.213
OR {22532}
( segid "PROT" and resid 78 and name HD2%)
( segid "PROT" and resid 34 and name HE% )
OR {22532}
( segid "PROT" and resid 78 and name HD2%)
( segid "PROT" and resid 68 and name HD% )
ASSI {22562}
( segid "PROT" and resid 102 and name HD1%)
(( segid "PROT" and resid 98 and name HB2 ))
3.300 2.700 2.200 peak 22562 weight 0.10000E+01 volume 0.83000E+00 ppm1 0.757 ppm2 3.101
OR {22562}
( segid "PROT" and resid 102 and name HD1%)
(( segid "PROT" and resid 106 and name HB2 ))
OR {22562}
( segid "PROT" and resid 102 and name HD1%)
(( segid "PROT" and resid 105 and name HB2 ))
OR {22562}
( segid "PROT" and resid 102 and name HD1%)
(( segid "PROT" and resid 82 and name HB1 ))
OR {22562}
( segid "PROT" and resid 102 and name HD1%)
(( segid "PROT" and resid 105 and name HB1 ))
OR {22562}
( segid "PROT" and resid 102 and name HD1%)
(( segid "PROT" and resid 85 and name HB2 ))
ASSI {22572}
( segid "PROT" and resid 115 and name HD1%)
(( segid "PROT" and resid 114 and name HA2 ))
3.000 2.200 2.200 peak 22572 weight 0.10000E+01 volume 0.14716E+01 ppm1 0.759 ppm2 4.052
OR {22572}
( segid "PROT" and resid 102 and name HD1%)
(( segid "PROT" and resid 28 and name HA ))
OR {22572}
( segid "PROT" and resid 115 and name HD1%)
(( segid "PROT" and resid 72 and name HA ))
OR {22572}
( segid "PROT" and resid 102 and name HD1%)
(( segid "PROT" and resid 56 and name HA ))
OR {22572}
( segid "PROT" and resid 115 and name HD1%)
(( segid "PROT" and resid 15 and name HA ))
ASSI {22692}
( segid "PROT" and resid 63 and name HD2%)
( segid "PROT" and resid 59 and name HE% )
2.700 1.800 1.800 peak 22692 weight 0.10000E+01 volume 0.24125E+01 ppm1 1.080 ppm2 1.317
OR {22692}
( segid "PROT" and resid 63 and name HD2%)
(( segid "PROT" and resid 19 and name HG1 ))
ASSI {22742}
( segid "PROT" and resid 18 and name HD1%)
(( segid "PROT" and resid 17 and name HB ))
3.600 3.200 1.900 peak 22742 weight 0.10000E+01 volume 0.48300E+00 ppm1 0.515 ppm2 4.277
OR {22742}
( segid "PROT" and resid 18 and name HD1%)
(( segid "PROT" and resid 73 and name HA ))
ASSI {22822}
( segid "PROT" and resid 73 and name HD1%)
(( segid "PROT" and resid 69 and name HA ))
3.100 2.400 2.400 peak 22822 weight 0.10000E+01 volume 0.10888E+01 ppm1 0.974 ppm2 4.103
OR {22822}
( segid "PROT" and resid 73 and name HD1%)
(( segid "PROT" and resid 67 and name HA ))
ASSI {22832}
( segid "PROT" and resid 14 and name HD1%)
(( segid "PROT" and resid 13 and name HA ))
3.200 2.600 2.300 peak 22832 weight 0.10000E+01 volume 0.10254E+01 ppm1 0.851 ppm2 4.225
OR {22832}
( segid "PROT" and resid 14 and name HD1%)
(( segid "PROT" and resid 115 and name HA ))
OR {22832}
( segid "PROT" and resid 14 and name HD1%)
(( segid "PROT" and resid 70 and name HB1 ))
ASSI {22852}
( segid "PROT" and resid 78 and name HD1%)
(( segid "PROT" and resid 109 and name HB2 ))
3.400 2.900 2.100 peak 22852 weight 0.10000E+01 volume 0.68210E+00 ppm1 0.097 ppm2 1.581
OR {22852}
( segid "PROT" and resid 78 and name HD1%)
(( segid "PROT" and resid 18 and name HB1 ))
OR {22852}
( segid "PROT" and resid 78 and name HD1%)
(( segid "PROT" and resid 115 and name HB2 ))
OR {22852}
( segid "PROT" and resid 78 and name HD1%)

```

```

(( segid "PROT" and resid 115 and name HG ))
ASSI {22912}
( segid "PROT" and resid 22 and name HD1% )
(( segid "PROT" and resid 63 and name HB2 ))
2.600 1.700 1.700 peak 22912 weight 0.10000E+01 volume 0.35385E+01 ppm1 1.108 ppm2 1.950
OR {22912}
(( segid "PROT" and resid 110 and name HG12 ))
(( segid "PROT" and resid 111 and name HB1 ))
ASSI {22952}
(( segid "PROT" and resid 110 and name HG12 ))
( segid "PROT" and resid 107 and name HD% )
3.200 2.600 2.300 peak 22952 weight 0.10000E+01 volume 0.10158E+01 ppm1 1.103 ppm2 7.230
OR {22952}
( segid "PROT" and resid 22 and name HD1% )
( segid "PROT" and resid 68 and name HD% )
ASSI {22972}
(( segid "PROT" and resid 98 and name HB2 ))
(( segid "PROT" and resid 99 and name HA ))
3.200 2.600 2.300 peak 22972 weight 0.10000E+01 volume 0.88740E+00 ppm1 3.094 ppm2 3.915
OR {22972}
(( segid "PROT" and resid 85 and name HB2 ))
(( segid "PROT" and resid 99 and name HA ))
ASSI {22982}
(( segid "PROT" and resid 98 and name HB2 ))
(( segid "PROT" and resid 30 and name HB1 ))
3.500 3.100 2.000 peak 22982 weight 0.10000E+01 volume 0.52590E+00 ppm1 3.082 ppm2 4.349
OR {22982}
(( segid "PROT" and resid 85 and name HB2 ))
(( segid "PROT" and resid 84 and name HA ))
ASSI {23002}
(( segid "PROT" and resid 109 and name HD1 ))
(( segid "PROT" and resid 112 and name HG2 ))
3.300 2.700 2.200 peak 23002 weight 0.10000E+01 volume 0.76170E+00 ppm1 1.417 ppm2 2.231
OR {23002}
(( segid "PROT" and resid 14 and name HG ))
(( segid "PROT" and resid 75 and name HG2 ))
ASSI {23062}
(( segid "PROT" and resid 115 and name HG ))
(( segid "PROT" and resid 110 and name HG12 ))
2.900 2.100 2.100 peak 23062 weight 0.10000E+01 volume 0.18772E+01 ppm1 1.569 ppm2 1.069
OR {23062}
(( segid "PROT" and resid 115 and name HG ))
(( segid "PROT" and resid 21 and name HG12 ))
ASSI {23112}
(( segid "PROT" and resid 78 and name HG ))
( segid "PROT" and resid 25 and name HG2% )
3.600 3.200 1.900 peak 23112 weight 0.10000E+01 volume 0.49400E+00 ppm1 0.692 ppm2 1.066
OR {23112}
(( segid "PROT" and resid 78 and name HG ))
( segid "PROT" and resid 22 and name HD2% )
ASSI {23352}
(( segid "PROT" and resid 80 and name HB2 ))
(( segid "PROT" and resid 54 and name HG1 ))
3.000 2.200 2.200 peak 23352 weight 0.10000E+01 volume 0.13200E+01 ppm1 1.939 ppm2 2.743
OR {23352}
(( segid "PROT" and resid 80 and name HB2 ))
(( segid "PROT" and resid 84 and name HB2 ))
ASSI {23462}
(( segid "PROT" and resid 9 and name HB1 ))
(( segid "PROT" and resid 8 and name HB1 ))
3.100 2.400 2.400 peak 23462 weight 0.10000E+01 volume 0.12491E+01 ppm1 1.884 ppm2 2.272
OR {23462}
(( segid "PROT" and resid 54 and name HG2 ))
(( segid "PROT" and resid 53 and name HB1 ))
OR {23462}
(( segid "PROT" and resid 54 and name HG2 ))
(( segid "PROT" and resid 53 and name HG1 ))
ASSI {23612}
(( segid "PROT" and resid 19 and name HB1 ))
( segid "PROT" and resid 63 and name HD2% )
3.300 2.700 2.200 peak 23612 weight 0.10000E+01 volume 0.79450E+00 ppm1 1.735 ppm2 1.082
OR {23612}
(( segid "PROT" and resid 19 and name HB1 ))
( segid "PROT" and resid 22 and name HD1% )
ASSI {23922}
(( segid "PROT" and resid 29 and name HG1 ))
( segid "PROT" and resid 101 and name HG2% )
3.500 3.100 2.000 peak 23922 weight 0.10000E+01 volume 0.51310E+00 ppm1 2.485 ppm2 1.021
OR {23922}
(( segid "PROT" and resid 29 and name HG1 ))
( segid "PROT" and resid 101 and name HD1% )
OR {23922}
(( segid "PROT" and resid 23 and name HG2 ))
( segid "PROT" and resid 22 and name HD2% )
ASSI {24012}
(( segid "PROT" and resid 42 and name HG2 ))
(( segid "PROT" and resid 39 and name HG2 ))
3.100 2.400 2.400 peak 24012 weight 0.10000E+01 volume 0.10550E+01 ppm1 2.255 ppm2 1.427
OR {24012}

```

```

(( segid "PROT" and resid 112 and name HG2 ))
(( segid "PROT" and resid 111 and name HG1 ))
OR {24012}
(( segid "PROT" and resid 112 and name HG2 ))
(( segid "PROT" and resid 113 and name HB% ))
OR {24012}
(( segid "PROT" and resid 112 and name HG2 ))
(( segid "PROT" and resid 109 and name HD1 ))
ASSI {24082}
(( segid "PROT" and resid 21 and name HB ))
(( segid "PROT" and resid 115 and name HD2% ))
3.500 3.100 2.000 peak 24082 weight 0.10000E+01 volume 0.53950E+00 ppm1 1.950 ppm2 0.756
OR {24082}
(( segid "PROT" and resid 21 and name HB ))
(( segid "PROT" and resid 115 and name HD1% ))
OR {24082}
(( segid "PROT" and resid 21 and name HB ))
(( segid "PROT" and resid 78 and name HB1 ))
ASSI {24102}
(( segid "PROT" and resid 21 and name HB ))
(( segid "PROT" and resid 24 and name HG2 ))
3.600 3.200 1.900 peak 24102 weight 0.10000E+01 volume 0.48680E+00 ppm1 1.951 ppm2 2.487
OR {24102}
(( segid "PROT" and resid 21 and name HB ))
(( segid "PROT" and resid 109 and name HE2 ))
ASSI {24162}
(( segid "PROT" and resid 77 and name HB1 ))
(( segid "PROT" and resid 54 and name HE% ))
3.500 3.100 2.000 peak 24162 weight 0.10000E+01 volume 0.51230E+00 ppm1 2.755 ppm2 2.010
OR {24162}
(( segid "PROT" and resid 77 and name HB1 ))
(( segid "PROT" and resid 80 and name HB1 ))
ASSI {24282}
(( segid "PROT" and resid 116 and name HB ))
(( segid "PROT" and resid 6 and name HE1 ))
3.300 2.700 2.200 peak 24282 weight 0.10000E+01 volume 0.80610E+00 ppm1 1.850 ppm2 2.995
OR {24282}
(( segid "PROT" and resid 116 and name HB ))
(( segid "PROT" and resid 118 and name HB1 ))
ASSI {24302}
(( segid "PROT" and resid 78 and name HB1 ))
(( segid "PROT" and resid 82 and name HE% ))
3.600 3.200 1.900 peak 24302 weight 0.10000E+01 volume 0.45690E+00 ppm1 0.738 ppm2 6.464
OR {24302}
(( segid "PROT" and resid 78 and name HB1 ))
(( segid "PROT" and resid 74 and name HD% ))
ASSI {24332}
(( segid "PROT" and resid 78 and name HB2 ))
(( segid "PROT" and resid 74 and name HE% ))
3.400 2.900 2.100 peak 24332 weight 0.10000E+01 volume 0.69100E+00 ppm1 0.472 ppm2 6.967
OR {24332}
(( segid "PROT" and resid 78 and name HB2 ))
(( segid "PROT" and resid 106 and name HD% ))
ASSI {24362}
(( segid "PROT" and resid 56 and name HB1 ))
(( segid "PROT" and resid 25 and name HG2% ))
2.800 2.000 2.000 peak 24362 weight 0.10000E+01 volume 0.23012E+01 ppm1 2.119 ppm2 1.058
OR {24362}
(( segid "PROT" and resid 56 and name HB1 ))
(( segid "PROT" and resid 22 and name HD2% ))
ASSI {24392}
(( segid "PROT" and resid 22 and name HB1 ))
(( segid "PROT" and resid 59 and name HE% ))
3.500 3.100 2.000 peak 24392 weight 0.10000E+01 volume 0.54020E+00 ppm1 2.130 ppm2 1.302
OR {24392}
(( segid "PROT" and resid 22 and name HB1 ))
(( segid "PROT" and resid 19 and name HG1 ))
ASSI {24862}
(( segid "PROT" and resid 115 and name HA ))
(( segid "PROT" and resid 6 and name HG1 ))
3.400 2.900 2.100 peak 24862 weight 0.10000E+01 volume 0.67380E+00 ppm1 4.256 ppm2 1.408
OR {24862}
(( segid "PROT" and resid 115 and name HA ))
(( segid "PROT" and resid 113 and name HB% ))
OR {24862}
(( segid "PROT" and resid 115 and name HA ))
(( segid "PROT" and resid 6 and name HG2 ))
ASSI {24932}
(( segid "PROT" and resid 34 and name HA ))
(( segid "PROT" and resid 31 and name HA ))
3.600 3.200 1.900 peak 24932 weight 0.10000E+01 volume 0.49270E+00 ppm1 5.003 ppm2 4.435
OR {24932}
(( segid "PROT" and resid 34 and name HA ))
(( segid "PROT" and resid 32 and name HA ))
ASSI {24952}
(( segid "PROT" and resid 6 and name HA ))
(( segid "PROT" and resid 6 and name HE1 ))
2.900 2.100 2.100 peak 24952 weight 0.10000E+01 volume 0.18164E+01 ppm1 4.375 ppm2 3.042
OR {24952}

```

```

(( segid "PROT" and resid 100 and name HA ))
(( segid "PROT" and resid 104 and name HE1 ))
ASSI {25012}
(( segid "PROT" and resid 109 and name HA ))
(( segid "PROT" and resid 21 and name HD1% ))
3.000 2.200 2.200 peak 25012 weight 0.10000E+01 volume 0.13055E+01 ppm1 4.075 ppm2 0.676
OR {25012}
(( segid "PROT" and resid 109 and name HA ))
(( segid "PROT" and resid 110 and name HG2% ))
ASSI {25392}
(( segid "PROT" and resid 46 and name HA ))
(( segid "PROT" and resid 49 and name HB ))
3.400 2.900 2.100 peak 25392 weight 0.10000E+01 volume 0.60870E+00 ppm1 3.501 ppm2 1.933
OR {25392}
(( segid "PROT" and resid 46 and name HA ))
(( segid "PROT" and resid 53 and name HG2 ))
ASSI {25412}
(( segid "PROT" and resid 20 and name HB1 ))
(( segid "PROT" and resid 17 and name HG2% ))
3.000 2.200 2.200 peak 25412 weight 0.10000E+01 volume 0.13236E+01 ppm1 4.097 ppm2 1.183
OR {25412}
(( segid "PROT" and resid 49 and name HA ))
(( segid "PROT" and resid 51 and name HB2 ))
ASSI {25482}
(( segid "PROT" and resid 49 and name HA ))
(( segid "PROT" and resid 87 and name HB2 ))
3.300 2.700 2.200 peak 25482 weight 0.10000E+01 volume 0.72460E+00 ppm1 4.123 ppm2 2.071
OR {25482}
(( segid "PROT" and resid 49 and name HA ))
(( segid "PROT" and resid 48 and name HB2 ))
OR {25482}
(( segid "PROT" and resid 53 and name HA ))
(( segid "PROT" and resid 54 and name HB1 ))
ASSI {25492}
(( segid "PROT" and resid 49 and name HA ))
(( segid "PROT" and resid 48 and name HG1 ))
3.000 2.200 2.200 peak 25492 weight 0.10000E+01 volume 0.14540E+01 ppm1 4.112 ppm2 2.383
OR {25492}
(( segid "PROT" and resid 20 and name HB1 ))
(( segid "PROT" and resid 23 and name HB1 ))
OR {25492}
(( segid "PROT" and resid 53 and name HA ))
(( segid "PROT" and resid 46 and name HB2 ))
OR {25492}
(( segid "PROT" and resid 53 and name HA ))
(( segid "PROT" and resid 55 and name HB1 ))
OR {25492}
(( segid "PROT" and resid 41 and name HA ))
(( segid "PROT" and resid 42 and name HG1 ))
ASSI {25642}
(( segid "PROT" and resid 21 and name HA ))
(( segid "PROT" and resid 20 and name HB1 ))
3.200 2.600 2.300 peak 25642 weight 0.10000E+01 volume 0.90030E+00 ppm1 3.800 ppm2 4.098
OR {25642}
(( segid "PROT" and resid 21 and name HA ))
(( segid "PROT" and resid 109 and name HA ))
ASSI {25682}
(( segid "PROT" and resid 58 and name HA ))
(( segid "PROT" and resid 61 and name HG1 ))
3.000 2.200 2.200 peak 25682 weight 0.10000E+01 volume 0.15120E+01 ppm1 3.883 ppm2 2.443
OR {25682}
(( segid "PROT" and resid 83 and name HA ))
(( segid "PROT" and resid 87 and name HG1 ))
ASSI {25902}
(( segid "PROT" and resid 76 and name HB% ))
(( segid "PROT" and resid 73 and name HD1% ))
3.100 2.400 2.400 peak 25902 weight 0.10000E+01 volume 0.11972E+01 ppm1 1.533 ppm2 0.984
OR {25902}
(( segid "PROT" and resid 76 and name HB% ))
(( segid "PROT" and resid 21 and name HG2% ))
ASSI {25912}
(( segid "PROT" and resid 76 and name HB% ))
(( segid "PROT" and resid 74 and name HB2 ))
3.700 3.400 1.800 peak 25912 weight 0.10000E+01 volume 0.39640E+00 ppm1 1.526 ppm2 2.462
OR {25912}
(( segid "PROT" and resid 76 and name HB% ))
(( segid "PROT" and resid 79 and name HG1 ))
ASSI {26132}
(( segid "PROT" and resid 113 and name HB% ))
(( segid "PROT" and resid 111 and name HB1 ))
3.500 3.100 2.000 peak 26132 weight 0.10000E+01 volume 0.58100E+00 ppm1 1.411 ppm2 1.932
OR {26132}
(( segid "PROT" and resid 113 and name HB% ))
(( segid "PROT" and resid 8 and name HB2 ))
OR {26132}
(( segid "PROT" and resid 113 and name HB% ))
(( segid "PROT" and resid 21 and name HB ))
ASSI {26152}
(( segid "PROT" and resid 93 and name HB1 ))

```

```

(( segid "PROT" and resid 94 and name HB1 ))
3.300 2.700 2.200 peak 26152 weight 0.10000E+01 volume 0.77140E+00 ppm1 3.864 ppm2 2.109
OR {26152}
(( segid "PROT" and resid 93 and name HB1 ))
(( segid "PROT" and resid 92 and name HB1 ))
ASSI {26482}
( segid "PROT" and resid 35 and name HE% )
(( segid "PROT" and resid 27 and name HB1 ))
3.400 2.900 2.100 peak 26482 weight 0.10000E+01 volume 0.70350E+00 ppm1 2.213 ppm2 4.052
OR {26482}
( segid "PROT" and resid 35 and name HE% )
(( segid "PROT" and resid 56 and name HA ))
OR {26482}
( segid "PROT" and resid 35 and name HE% )
(( segid "PROT" and resid 28 and name HA ))
OR {26482}
( segid "PROT" and resid 35 and name HE% )
(( segid "PROT" and resid 60 and name HB2 ))
ASSI {26502}
( segid "PROT" and resid 81 and name HG1% )
( segid "PROT" and resid 56 and name HD2% )
2.300 1.300 1.300 peak 26502 weight 0.10000E+01 volume 0.62878E+01 ppm1 0.506 ppm2 0.677
OR {26502}
( segid "PROT" and resid 81 and name HG1% )
(( segid "PROT" and resid 78 and name HG ))
ASSI {26512}
( segid "PROT" and resid 116 and name HD1% )
(( segid "PROT" and resid 6 and name HG1 ))
2.800 2.000 2.000 peak 26512 weight 0.10000E+01 volume 0.22365E+01 ppm1 0.828 ppm2 1.429
OR {26512}
( segid "PROT" and resid 116 and name HD1% )
(( segid "PROT" and resid 6 and name HG2 ))
OR {26512}
( segid "PROT" and resid 116 and name HD1% )
(( segid "PROT" and resid 111 and name HG1 ))
ASSI {26702}
( segid "PROT" and resid 18 and name HD2% )
( segid "PROT" and resid 75 and name HE% )
3.500 3.100 2.000 peak 26702 weight 0.10000E+01 volume 0.52720E+00 ppm1 -0.158 ppm2 2.088
OR {26702}
( segid "PROT" and resid 18 and name HD2% )
(( segid "PROT" and resid 22 and name HB1 ))
OR {26702}
( segid "PROT" and resid 18 and name HD2% )
(( segid "PROT" and resid 8 and name HG1 ))
ASSI { 345}
(( segid "PROT" and resid 87 and name HB2 ))
(( segid "PROT" and resid 87 and name HG2 ))
3.100 2.400 2.400 peak 345 weight 0.10000E+01 volume 0.11110E+01 ppm1 2.075 ppm2 2.246
OR { 345}
(( segid "PROT" and resid 112 and name HB1 ))
(( segid "PROT" and resid 112 and name HG2 ))
ASSI { 365}
(( segid "PROT" and resid 87 and name HB1 ))
(( segid "PROT" and resid 86 and name HA ))
3.300 2.700 2.200 peak 365 weight 0.10000E+01 volume 0.81740E+00 ppm1 2.169 ppm2 4.226
OR { 365}
(( segid "PROT" and resid 87 and name HB1 ))
(( segid "PROT" and resid 83 and name HB ))
ASSI { 395}
(( segid "PROT" and resid 112 and name HB1 ))
(( segid "PROT" and resid 108 and name HA ))
3.400 2.900 2.100 peak 395 weight 0.10000E+01 volume 0.70760E+00 ppm1 2.075 ppm2 4.226
OR { 395}
(( segid "PROT" and resid 87 and name HB2 ))
(( segid "PROT" and resid 86 and name HA ))
ASSI { 485}
(( segid "PROT" and resid 19 and name HD1 ))
(( segid "PROT" and resid 19 and name HE1 ))
3.000 2.200 2.200 peak 485 weight 0.10000E+01 volume 0.13981E+01 ppm1 1.618 ppm2 2.941
OR { 485}
(( segid "PROT" and resid 111 and name HD1 ))
(( segid "PROT" and resid 111 and name HE1 ))
ASSI { 176}
( segid "PROT" and resid 107 and name HD% )
(( segid "PROT" and resid 111 and name HB1 ))
2.900 2.100 2.100 peak 176 weight 0.10000E+01 volume 0.23424E+01 ppm1 7.234 ppm2 1.923
OR { 176}
( segid "PROT" and resid 107 and name HD% )
(( segid "PROT" and resid 103 and name HG2 ))
OR { 176}
( segid "PROT" and resid 105 and name HD% )
(( segid "PROT" and resid 104 and name HB1 ))

```